

## Course No: CH24101CR Title: Inorganic Chemistry (04 Credits)

Max. Marks: 100	<b>Duration: 64 Contact hours</b>		
Continuous Assessment: 20 marks	End Term Exam: 80 Marks		
Course outcomes: After studying this course, the students will be able to			

know about the thermodynamic stability of metal complexes and learn the stepwise formation of complexes and their stability constant.

- discuss the properties of coordination compounds and explain bonding in Octahedral, Square-planar and Tetrahedral complexes using Molecular Orbital Theory.
- > familiarize students about synergic nature of bonding in metal carbonyl complexes and the nature of interaction in other  $\pi$ -acceptor ligands and metal clusters.
- understand the properties of Lanthanide elements and their complexation behavior with selected ligands. Applications of lanthanide complexes as NMR shift reagents and MRI contrast agents.

#### **Unit-I Metal-Ligand Equilibria in Solution**

## nstants (normal and abnormal trends) Mechanisms of selected

Stepwise and overall formation constants (normal and abnormal trends). Mechanisms of selected complexation processes. d<sup>n</sup> configuration and lability and stability of uncommon oxidation states.

(07 hr) Metal Chelates: Characteristics, Chelate effect and the factors affecting stability of metal chelates. Ligand preorganization, Tertiary phosphine as ligand. (03 hr)

Determination of formation constants by pH- metry and spectrophotometry. Structural (ionic radii) and thermodynamic (hydration and lattice energies) effects of crystal field splitting. Jahn-Teller distortion, spectrochemical series. (06 hr)

#### **Unit-II Bonding Models in Coordination Compounds**

Experimental Evidence in favor of Metal Ligand Orbital Overlap; Adjusted crystal field theory. (04 hr)

Molecular orbital theory of bonding in octahedral complexes:- composition of ligand group orbitals; molecular orbitals and energy level diagram for sigma bonded  $ML_6$ ; Effect of pi-bonding (Pi-donor and Acceptor Ligands). (08 hr)

Molecular orbital and energy level diagram for bonding in Square-planar and Tetrahedral complexes. (04 hr)

#### (16 Contact hours)



#### Unit-III Bonding in Pi-acid metal complexes and Metal clusters (16 Contact hours)

<u>Transition Metal Carbonyls</u>: Carbon monoxide as Pi-acid ligand, structure and bonding of monoand poly-nuclear carbonyls. Vibrational spectra of metal carbonyls. Structure and bonding of transition metal nitrosyls, dinitrogen and dioxygen complexes (comparative account).

(10 hr)

(16 Contact hours)

**Bonding in Metal clusters:** Factors favoring metal-metal bond, bonding in di- and trinuclear metal clusters, Cotton rationale and quadruple bonding, selected examples of bonding in hetero-polymetallates (06 hr)

#### **Unit-IV Coordination Chemistry of Lanthanides**

Electronic Configuration and Oxidation states. f-orbital's. Coordination numbers, stereochemistry and stability of lanthanide Complexes. (05 hr)

Selected examples of lanthanide complexes with nitrate,  $\beta$ -Diketonate, crown Ether and porphyrin type ligands. Homo and hetero dinuclear coordination compounds, coordination polymers of lanthanide ions (elementary idea). (05 hr)

Properties and Applications of Lanthanides: Utility of Lanthanide Complexes as Sensory Probes, Lasers, NMR Shift Reagents and Contrast Agents in Magnetic Resonance Imagining (MRI).

(**06 hr**)

#### **Books Recommended:**

- 1. Inorganic Chemistry; Weller, Overton, Rourke, Armstrong; 6th Edn.; Oxford University Press; 2015
- 2. Chemistry of the Elements; 2<sup>nd</sup> Edn; N. N. Greenwood, A. Earnshaw; Elsevier; 2014.
- 3. Inorganic Chemistry; 3<sup>rd</sup>Edn; D. F. Shriver; P. W. Atkins; Oxford; 1999.
- 4. Concise Inorganic Chemistry; J. D. Lee; 5thEdn.; Black Well Publishing; 2006
- 5. Principles of Inorganic Chemistry; 1<sup>st</sup>edn.; Brain W. Pfennig; Wiley; 2015.
- 6. Advanced Inorganic Chemistry; 3<sup>rd</sup>, 5<sup>th</sup> and 6<sup>th</sup>edn; F. A. Cotton, G. Wilkinson; Wiley; Sixth edition (1 January 2007).
- 7. Advanced Inorganic Chemistry, G. H Bailey, W. Briggs, Legare Street Press (9 September 2021).
- 8. Inorganic Chemistry; 4th edn; J. E. Huheey; E. A. Keiter; Harper Collins; 2009.
- 9. Inorganic Chemistry; K.F. Purcell, J.C Kotz; Cengage (1 January 2010)
- 10. Lanthanide and Actinide Chemistry; Simon Cotton; 2nd Revised Edn.; John Wiley & Sons: West Sussex, England; 2006.
- 11. The Chemistry of the Lanthanides: Pergamon Texts in Inorganic Chemistry, T. Moeller, Pergamon (22 October 2013).
- 12. Coordination Chemistry; D. Banerjea; Asian Books 2009
- 13. Comprehensive coordination chemistry, B. J. Hathaway, pergamon press, oxford, 1987.
- 14. Inorganic Chemistry, G. Wulfsberg, Viva Books (1 January 2018).



## Course No: CH24102CR **Title: Organic Chemistry (04 Credits)**

Max. Marks: 100	<b>Duration: 64 Contact hours</b>
Continuous Assessment: 20 marks	End Term Exam: 80 Marks

**Course outcomes:** On completion of the course, the student should be able to:

- > Recognize the key reactive intermediates their stability and determination of reaction mechanism.
- ➢ Grasp different aspects of stereochemistry.
- > Understand the different types of substitution reaction mechanisms in both aliphatic and aromatic compounds and elimination reactions.

**Unit-I: Basic Organic Chemistry and Reactive intermediates** (16 Contact hours)

Fundamentals of Organic Chemistry: Electronic displacement effects applicable to reaction mechanism: Inductive, conjugative/resonance and hyperconjugative effects. Cross conjugation.

Rules for writing resonance structures. Application of organic acids and bases. Nucleophiles and electrophiles. (06 hrs)

Aromaticity: Huckel rule and concept of aromaticity, Molecular orbital diagram of annulenes, Frost diagram. Anti and Homoaromaticity. (04 hrs)

Annulenes: Systems with  $\pi$ -electron numbers other than six (2,4,8,10 and more than ten  $\pi$ electron systems), Aromaticity of hetero annulenes. Aromaticity in fused ring systems. (03 hrs) Reactive Intermediates: Generation, Structure, fate and stability of Carbocations (Classical and Non- Classical), Carbanions, Free radicals, Carbenes, Nitrenes, Arynes and Radical ions.(03 hrs)

#### **Unit-II: Stereochemistry of Organic Compounds**

Stereoisomerism: Definition, Classification, Configuration: D L & R S. (02 hrs) *Chirality*: Molecules with carbon and non-carbon atom as chiral centre. Chirality in adamantanes. Chirality in absence of chiral carbons: axial chirality (allenes, biphenyls spiranes, atropoisomeric) planar and helical chirality(P & M). (07 hrs)

Topicity and cyclo-stereoisomerism: Topicity of ligands and faces. Conformations and conformational analysis of cycloalkanes: cyclopropane, cyclobutane and cyclohexane. Conformations of disubstituted cyclohexanes (1,2; 1,3 & 1,4)), disubstituted conformations of cyclohexenes, cyclohexanones, decalins and azodecalins, conformation of sugars. (07 hrs)

#### **Unit-III: Physical Organic Chemistry and Reaction Mechanism-I** (16 Contact hours)

Determination of Reaction Mechanism: Thermodynamic and kinetic evidences. Isotope labelling and kinetic isotope effect, isolation of product, Identification of intermediates Acid-base catalysis: General and specific. (03 hrs)

Aliphatic Nucleophilic Substitutions: S<sub>N</sub>2, S<sub>N</sub>1, S<sub>N</sub>i and Neighbouring group participation Stereochemistry of S<sub>N</sub>2 and S<sub>N</sub>1 reactions. Nucleophilic substitution at allylic, benzylic, and vinylic carbons. Nucleophilic substitutions in biological systems. (08 hrs)



<u>Elimination reactions</u>: Mechanism and stereochemical implications of E1, E2, E1cB and E2C elimination reactions. Comparison between substitution and elimination reactions. Shapiro reaction. (05 hrs)

#### **Unit-IV: Reaction Mechanism-II**

#### (16 Contact hours)

Aromatic Electrophilic Substitution: General mechanism, Orientation (theoretical/spectral evidences) and reactivity of di-substituted benzene rings. Ipso attack, Reversal of Friedal Craft (FC) alkylation. Synthetic application of F.C acylation and nitration reactions (Toluene to nitro – benzoic acids, synthesis of ortho and para nitro anilines). (08 hrs) Aromatic Nucleophilic substitution: Discussion of different mechanisms (S<sub>N</sub>1, S<sub>N</sub>Ar, Benzyne and S<sub>RN</sub>1). Mechanisms of von- Richter, Sommelet-Hauser and Chichibabin reaction. (03 hrs) Free Radical Substitution: Free radical substitution mechanisms. Neighbouring Group Assistance in free radical reactions. Factors affecting radical substitutions. Auto-oxidation, Hunsdiecker reactions. (05 hrs)

## **Books Recommended:**

- March's Advanced Organic Chemistry Reactions, Mechanism and Structure, 6<sup>th</sup> Ed., Smith, M.B. (Wiley-2014)
- 2. Organic Chemistry 8th Ed. F. A. Carey and Robert M. Giuliano (McGraw Hill-2012).
- 3. Reaction Mechanism in Organic Chemistry RevisedEd., S.M. Mukherjee and S.P. Singh. (Macmillan- 2017).
- 4. Organic Chemistry 2<sup>nd</sup> Ed., J. Hornback. (Brooks/Cole- 2006).
- 5. Organic Chemistry, 5<sup>th</sup> Ed., John McMurry. (Brooks/Cole-2000).
- 6. Advanced Organic Chemistry, 5<sup>th</sup> Ed., F.A Carey & R.J Sundberg (Springer-2007).
- 7. Organic Chemistry, 2<sup>nd</sup> Ed., Jonathan Clayden (OUP-2016).
- 8. Organic Chemistry, 11<sup>th</sup> Ed., Solomons, T.W.G., (Wiley-2015).
- 9. Organic chemistry, Morrison, Boyd and Bhattacharya. 7th Ed. Pearson-2013.
- 10. Stereochemistry of Organic Compounds 2<sup>nd</sup> Ed., D. Nasipuri. (New Age Inter.- 2008)
- 11. Stereochemistry of Carbon Compounds E.L.Eliel. (TMH -2007)
- 12. Stereochemistry of Organic Compounds 7th Ed. P.S. Kalsi. (New Age Inter.- 2012).

## Course No: CH24103CR Title: Physical Chemistry (04 Credits)

Max. Marks: 100	Duration: 64 Contact hours
Continuous Assessment: 20 marks	End Term Exam: 80 Marks

**Course outcomes:** After learning the contents of this course, the students shall:

- > Learn basics of some mathematical concepts and their use in chemical investigations
- ➤ be able to understand the genesis of quantum mechanics and its basic formulations for understanding the microscopic world.
- learn to solve the Schrodinger equation to evaluate energy of simple systems with or without potential energy.
- > learn what are fast reactions and how kinetic investigations are carried out for such reactions.
- > understand why chemical reactions are associated with energy barriers
- learn about the basic approximations, and theoretical predictions from different reaction rate theories like collision theory, transition state theory, theories of unimolecular reactions and linear free energy relations.
- be able to make predictions about the rate constants of reactions using different reaction rate theories and free energy relations and compare the same with experimental data
- ▶ be able appreciate the need and role of solvent in chemical reactions

#### **Unit-I Mathematics for Chemists**

Functions and equations:Functions in chemical context, Representation of single variablefunctions; tabular and graphical. Special mathematical functions and their properties (Exponential,logarithmic and Trigonometric), Solving polynomial equations in chemistry.*Differentiation*:The concept, rules and applications in chemistry (Finding maxima, minima andinflection points). Simple differential equations*Integration*:The concept, rules and applications in chemistry.*Matrices*:The concept, matrices with special properties, addition and multiplication of matrices,operations on matrices, solving linear equations with matrices.(03 hrs)Mean and standard deviation, Normal distribution function.

#### **Unit-II Quantum Chemistry-I**

Schrodinger equation: time-independent and time-dependent. Postulates of quantum mechanics.Operator concept, quantum mechanical operators in spherical polar co-ordinate system, some<br/>properties of quantum mechanical operators.**Exactly solvable problems:**<br/>harmonic oscillator & the rigid rotator. Tunneling effect.**(06 hrs)** 

Born-Oppenheimer Approximation, Solution of the Hydrogen-like atom problem, radial and angular wave functions. (03 hrs)

#### **Unit-III Chemical kinetics-I**

<u>Theories of Chemical Reactions</u>: Arrhenius and Collision theory, Potential energy surfaces, Activated complex theory of reaction rates, statistical & thermodynamic formulations, comparison with collision theory. (07 hrs)

# (16 Contact hours)

(16 Contact hours)



Unimolecular reactions:Lindman, Hinshelwood, RRK and RRKM theories.(04 hrs)Structure Reactivity Relationships:Linear Free-Energy Relationships (LFER), Bronstedequation, Bell-Evans-Polanyi equation, Hammet and Taft relationships. Hammond postulates, thereactivity-selectivity principle.(05 hrs)

#### **Unit-IV Chemical kinetics-II**

<u>Surface Reactions</u>: Unimolecular & bimolecular surface reactions [Langmuir-Hinshelwood & Langmuir- Riedel mechanism], classical & statistical treatments. (04 hrs)

<u>Reactions in solutions</u>: Effect of solvent on reaction rates, Diffusion controlled reactions (partial & full microscopic diffusion control), Ionic Reactions; Single & double sphere models of ionic reactions, effect of ionic strength. (06 hrs)

<u>Chain reactions</u>: Explosive reactions, Polymerization reactions (free radical, cationic and anionic) (03 hrs)

*Fast reactions:* General features of fast reactions, study of fast reactions by flow method, relaxation method and flash photolysis. (03 hrs)

## **Books Recommended:**

- 1. Maths for Chemists, Martin Cockett & Graham Dogget, 2nd Edition, RSC Publishing, 2012.
- 2. Maths for Chemistry, A Chemist's Toolkit of Calculations, Paul Monk & Lindsey J Munro, 3rd Edition, Oxford University Press, 2021.
- 3. Atkins' Physical Chemistry, Peter William Atkins, Julio De Paula, & James Keeler, 12th Edition, Oxford University Press, 2023
- 4. Physical Chemistry- A Molecular Approach D. A. McQuarie& J. D. Simon, University Science Books, 1997.
- 5. Introduction to Quantum chemistry A. K. Chandra, TataMcGraw Hill, 1997.
- 6. Quantum Chemistry Ira. N. Levine, 7th Edition, Pearson, 2014.
- 7. Quantum Chemistry, R. K. Prasad, 2nd Edition, New Age Publishers, 2001.
- 8. Chemical Kinetics, K. J. Laidler, 3rd Edition, Pearson, 1987.
- 9. Chemical Kinetics and Reaction Dynamics, Paul L. Houston, Dover Publications, INC., Mineola, New York, 2001.
- 10. Chemical Kinetics and Dynamics, J. I. Steinfeld, J. S. Francisco, W.L. Hase, Prentice Hall, 1989
- 11. Chemical Kinetics and Catalysis, R.I. Masel, Wiley, 2001
- 12. Chemical Kinetics: From Molecular Structure to Chemical Reactivity, Luis G Arnaut, Sebastiao Jose Formosinho, Hugh Burrows, Elsevier, 2007.



## **Course No: CH24104CR**

## **Title: Environmental Chemistry and Analytical Monitoring (02 Credits)**

Max. Marks: 50	<b>Duration:</b>	32	Contact	hours
<b>Continuous Assessment: 10 marks</b>	End Term <b>F</b>	Exam:	40 Marks	

**Course outcomes:** After studying this course, the students will be able

- to understand the chemistry in the natural segments of environment (Atmosphere and Hydrosphere).
- > to understand the significance and skill of analytical monitoring.
- to have an understanding of various analytical methods for assessment of water quality and water treatment technologies.

#### **Unit-I Chemistry of the Environment**

*Atmosphere:* Vertical profile of the atmosphere; tropospheric reactivity patterns; stratospheric chemistry (Chapman mechanism and ozone depletion). Chemistry and control of Green house effect, Acid rain and Photochemical smog. (05 hrs)

*<u>Hydrosphere</u>*: Factors determining composition of water bodies (acid-base, Distribution diagram), thermal-stratification, pE concept and Pourbiax diagram and oxygen sag curve).

Water treatment: Chlorination, Ozonation and UV radiation.

Water treatment techniques: adsorption, advanced oxidation processes and Photo catalysis by nanomaterials. Bioremediation (04 hrs)

#### **Unit-II Environmental Monitoring**

Choice of methods for determining trace metals (As,Cd, Hg,Pb and Se). Analytical methods for measuring air pollutants: General aspects, Sampling and methods of analyses. Water quality parameters: Dissolved oxygen, metals, chloride, phosphate and nitrate. Water quality standards.

(05 hrs)

Analytical methods for determining water quality parameters: DO, BOD and COD. (**05 hrs**) Continuous monitoring instruments as analytical tools for real time monitoring of pollutants (NDIR, GC-MS, Chemiluminescence and Spectrophotometry). Water Analysis Methods: Spectrophotometry (Chromogenic step) and Electrochemical methods. (**06 hrs**)

## **Books Recommended**

- 1. Environmental Chemistry; Nigel. J. Bunce; Wurez Publishers; 1991.
- 2. Environmental Chemistry; 2<sup>nd</sup>edn; Colin Baird; Freeman & Co; 1991.
- 3. Environmental Chemistry; A. K. De; Wiley Eastern; 1995.
- 4. Environmental pollution Analysis; S. M. Khopkar; new age publishers; 2nd edition (2020).
- 5. Principles of Environmental Chemistry, J. Girard, Jones and Bartlett Publishers, Inc; 3<sup>rd</sup> edition (2013).
- 6. Environmental chemistry, S. E Manahan, CRC Press; 5<sup>th</sup> edition onwards (2022)
- 7. Environmental pollution; B. K. Sharma & H. Kaur; Goel Publishers;1996.

#### (16 Contact hours)

(06 hrs)



- 8. Systematic methods of water quality parameters analysis: analytical methods, V. R Gopinath, Partridge Publishing Singapore (2021)
- The Quality of Air (Comprehensive Analytical Chemistry, M. d. Guardia, S. Armenta, Elsevier; 1<sup>st</sup> edition (2016)
- 10. Chemistry for environmental engineering and science, C. Sawyer, P. McCarty, G. parkin, McGraw-Hill Education; 5<sup>th</sup> edition (16 September 2002).
- 11. Principles of Environmental Chemistry, J. E. Girard, Jones & Bartlett Learning; 3rd edition (2013)
- 12. Environmental Chemistry, C. Baird, M. Cann, W. H. Freeman & Co Ltd; 5th ed. 2012 edition 2012)

## Course No: CH24105DCE

## **Title: Laboratory Course in Chemistry-I (04 Credits)**

Max. Marks: 100	Duration: 128 Contact hours
Continuous Assessment: 20 marks	End Term Exam: 80 Marks

**Course outcomes:** The main outcomes of the course are:

- to engage students with a series of well-planned experiments wherein they are expected to learn how to plan and conduct experiments in a physical chemistry lab.
- to carry out hands-on experiments to know how the data generated depicts the variation of various physical properties with the dependable parameters.
- to interpret the generated data through various theories to understand applications and relevance of physical methods to understand and explore the chemical systems.

#### A. Viscometery

- 1. Investigation of variation of viscosity with conc. and determination of unknown concentration and the radius of solute molecule by viscosity measurement.
- 2. Determination of Mol. Mass of a Polymer (Polyvinyl alcohol) using viscosity method.
- 3. Biodiesel and its viscosity measurement.

#### **B.** Calorimetry

- 1. Determination of heat of neutralization of a strong acid with a strong base.
- 2. Determination of heat of neutralization of a weak acid with a strong base.
- 3. Determination of the specific heat of a metal.

#### C. Phase Equilibria

- 1. Investigate the mutual solubility of phenol and water at various temperatures and hence determine the critical solution temperature of phenol-water system.
- 2. Study the effect of addition of NaCl/Succinic acid on the critical solution temperature of Phenol-Water System.
- 3. Investigate the solubility of three component systems and hence draw a tie line on binodal curve.

#### **D.** Chemical Kinetics

- 1. Determination of order of reaction between  $K_2S_2O_8$  and KI by Initial rate method using clock reaction.
- 2. Compare the effect of ionic strength on the rate constant of persulphate-iodide reaction and iodide-Fe(III) reactions using clock method.
- 3. Determination of the rate constant of inversion of cane sugar catalyzed be HCl using polarimeter.



#### E. Conductometry

- 1. Determination of the composition of a mixture of HCl and  $CH_3COOH$  by titration with standard NaOH.
- 2. Precipitation titration of BaCl<sub>2</sub> and K<sub>2</sub>SO<sub>4</sub>/ (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub>
- 3. Estimation of the concentrations of  $H_2SO_4$ ,  $CH_3COOH$  and  $CuSO_4$  in a mixture.

#### F. Potentiometry

- 1. Determination of strength and pKa value of weak acid by titration with an alkali using quinhydrone electrode.
- 2. Titration of Fe (II) vs.  $K_2Cr_2O_7$  and determination of standard redox potential of Fe<sup>2+</sup> /Fe<sup>3+</sup>.
- 3. Precipitation titration of KCl, KBr, KI and their mixture with AgNO<sub>3</sub>.

#### G. pH-metry

- 1. Determination of pKa values of a tribasic acid by titration with an alkali.
- 2. Determination of  $H_3PO_4$  content in a given sample of Coca-Cola.
- 3. Determination of degree of hydrolysis of a given salt using pH-metry.

#### H. Spectrophotometry

- 1. Determination of composition of a binary mixture of  $K_2Cr_2O_7$  and  $KMnO_4$  or Cobalt (II) and Nickel (II) ions.
- 2. To study the complexation reaction between Fe(III) & salicylic acid.
- 3. Recording Absorption spectra of a series of conjugated dyes-Application of the particle in one dimensional box.

## **Books Recommended:**

- 1. Practical Physical Chemistry, Findley, Kitchener, Longman, 1977.
- 2. Advanced Practical Physical Chemistry, Yadav, Goel Pub, 1994.
- 3. Experiments in Physical Chemistry, 5th ed., Schoemakeret al., MGH, 1989.



## Course No: CH24106DCE Title: Symmetry and Group Theory (02 Credits)

# Max. Marks: 50Duration: 32 Contact hoursContinuous Assessment: 10 marksEnd Term Exam: 40 Marks

#### **Course outcomes:**

- > Identification of symmetry elements and assignment of point groups to the molecules.
- Understanding of the fundamental aspects i.e. symmetry elements, operations, point groups, and character tables, and their application to electronic, infra-red and Raman spectroscopy.
- Construction and interpretation of Character Tables.

#### **Unit-I Molecular Symmetry**

Molecular Symmetry - Symmetry elements and operations: Identity, rotation axis, reflection plane, inversion centre, improper rotation axis. Combination of symmetry operations. Group multiplication tables. Symmetry groups. (08 hrs)

Symmetry Classification of Molecules: Point groups.Schoenflies notation of point groups.Identification of molecular point groups.(06 hrs)

Space Symmetry: Translation, screw axis, glide plane. Introduction to space groups. (03 hrs) Matrices and their combination, block factored matrices, Matrix representation of symmetry operations. (03 hrs)

#### **Unit-II Character Tables and Spectroscopy**

The Great Orthogonality Theorem: Elementary idea and consequences. Properties of irreducible representations (IRs), Mullikan symbols for IRs. (03 hrs) Character table-construction of character tables for  $C_2v$ ,  $C_3v$  and  $C_4v$  point groups. (05 hrs) Applications of group theory to IR and Raman spectroscopy. Degrees of freedom/molecular

motions-Vibrational motions. Selection rules. Symmetry of IR and Raman active normal<br/>vibrational modes of AB2, AB3, AB4, AB5, and AB6 type molecules.(04 hrs)Symmetry considerations of electronic transitions.(02 hrs)

Applications of symmetry to molecular chirality, polarity and hybridization. (02 hrs)

## **Books Recommended**

1. Chemical Applications of Group Theory; 2nd edn.; F.A.Cotton; Wiley Eastern;(1994)

2. Molecular Symmetry and Group Theory; L. Carter; Wiley; 1998.

3. Symmetry and Spectroscopy of Molecules; K. Veera Reddy; New Age 1998.

4. Inorganic Chemistry, Principles of structure and reactivity; 4th Edition; James E.Huheey,

Ellen A. Keiter and Richard L. Keiter. Pearson Education Inc

5. Physical Methods for Chemists; R. S. Drago; 2nd edn; Saunders; 1992.

#### (16 contact hours)

(16 Contact hours)

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## **Course No: CH24107DCE**

## **Title: Infrared, Raman and Electronic Spectroscopy (02 Credits)**

#### Max. Marks: 50 Continuous Assessment: 10 marks

#### **Duration: 32 Contact hours End Term Exam: 40 Marks**

Course outcomes: The outcomes include:

- to provide the basic and advanced level understanding about Infrared, Raman, and electronic spectroscopies to the students of MSc 1st semester from a Physico-Chemical perspective.
- to learn the conceptual basis of the subject and to train in problem solving and applications of spectroscopy to various chemical systems.
- to understand the spectroscopy to the level where students identify the spectroscopy as a basic and important experimental tool to probe the chemical systems.

#### Unit-I

## (16 Contact hours)

#### **Fundamentals of Spectroscopy**

Interaction of electromagnetic radiation with matter, transition probability, transition dipole moment integral, selection rules, Natural spectral line width and broadening of spectral lines - Doppler and Collision effects. (03 hrs)

Intensity of spectral lines, Fourier Transform Spectroscopy.

Beer Lambert Law and its application in determining the concentration of analytes. (03 hrs)

#### **Infrared Spectroscopy**

Linear-harmonic oscillator- classical and quantum treatment of vibrations, vibrational energies of diatomic molecules, zero-point energy, force constant and bond strength, anharmonicity, Morse potential energy levels. Fundamental bands, overtones and hot bands. Vibration- rotation spectra of diatomic molecules; P, Q and R branches. (8 hrs)

Vibrations of polyatomic molecules: Normal vibrational modes, selection rules; combination and difference bands. Group frequencies and finger print region. (2 hrs)

#### Unit-II

#### (16 Contact hours)

#### Raman Spectroscopy

Classical concept of Raman scattering, molecular polarizability, rotational, vibrational, and vibrational-rotational Raman spectra. Selection rules; rule of mutual exclusion. Applications. (06 hrs)

#### **Electronic and Photoelectron Spectroscopy**

Molecular Electronic Spectroscopy:Vibronic transitions, Franck-Condon principle, electronicspectra of polyatomic molecules, Different types of electronic transitions; nomenclature,symmetry labels of electronic states--spectraofformaldehyde, Symmetry selection rules,molecular Term Symbol (Elementary Idea).(06 hrs)

<u>*Photoelectron Spectroscopy:*</u> Basic principles- photoionization process; ionization energies; Koopman's theorem. Photoelectron spectra of simple molecules  $(N_2, O_2)$ . **(04 hrs)** 



## **Books Recommended**

- 1. Molecular Spectroscopy; 2<sup>nd</sup> edn; J L. McHale; CRC Press 2015.
- 2. Infrared and Raman Spectroscopy; Principles and Spectral Interpretation; 2<sup>nd</sup> edn.; P. Larkin; Elsevier; 2011.
- 3. Introduction of Spectroscopy; 4<sup>th</sup> edn.; D.L. Pavia, G. M. Lampman, G. S. Kriz, J. Vyvan; Cengage Learning, 2008.
- 4. Introductory Raman Spectroscopy; J. R. Ferraro, K. Nakamoto & C. W Brown; 2nd edn; Academic Press 2005.
- 5. Modern Spectroscopy; J.M. Hollas; Wiley; 2004..
- 6. Physical Methods for Chemists; R.S. Drago; 2<sup>nd</sup> edn; Saunders; 1992.
- 7. Fundamentals of Molecular Spectroscopy; C.N. Banwell, E.M. McCash; 4th edn; Tata McGraw Hill; 1994.
- 8. Physical chemistry; P. W. Atkins; 6th edition; Oxford University Press; 1998.
- 9. Electronic Absorption Spectroscopy and related techniques; D N Sathyanarayna; Universities Press.
- 10. Theory and Applications of Ultraviolet Spectroscopy; H.H. Jaffe, M. Orchin; Wiley; 1962.
- 11. Molecular Spectroscopy; 1<sup>st</sup> Edn; J.L. Mchale; Prentice Hall; 1999.
- 12. Structural Methods in Inorganic Chemistry; 2<sup>nd</sup> Edn; E.A.V. Ebsworth, D.W.H. Rankin, S. Cradock; Blackwell; 1991.
- 13. Molecular Spectroscopy: Quantum to Spectrum, Amita Dua and Prateek Tyagi, Atlantic Publishers and Distributors (P) Ltd, 2022.



## Course No: CH24001GE

## **Title: Surfactants and their Applications (02 Credits)**

#### Max. Marks: 50

#### Duration: 32 Contact hours End Term Exam: 40 Marks

**Continuous Assessment: 10 marks** 

**Course outcomes:** After learning the contents of this course, the students shall:

- > be familiar with the types of surfactants, their aggregation behavior and structure of aggregates.
- ➢ be familiar with the applications of the surfactant systems in da-to-day life, industries, catalysis, environment and pharmaceuticals.

#### **Unit-I Surfactants and their properties**

<u>Surfactants and Micelles:</u> Classification of surfactants, solubility of surfactants: Kraft temperature and cloud point, Micellization of surfactants: critical micelle concentration (cmc), aggregation number, counterion binding, factors affecting cmc in aqueous media. Thermodynamics of micellization: mass action model only. Structure and shape of micelles: geometrical consideration of chain packing. (10 hrs) <u>Micellar Solubilization:</u> Introduction, factors affecting micellar solubilization: nature of surfactant/solubilizate, effect of additive and temperature. Solubilization of drugs into micelles and its importance in drug delivery systems and controlled release. (6 hrs)

#### Unit-II Micellar catalysis and mixed-Surfactant Systems

<u>Micellar Catalysis:</u> Introduction of reactions in micellar media. Examples of micellar catalysis for hydrolysis, oxidation and reduction reactions (8 hrs)

*Mixed Surfactant systems:* Mixed micelle formation, synergism, Clint and Rubingh models of mixed micelle formation. Importance and practical applications of mixed surfactant systems. (8 hrs)

## **Books Recommended**

- 1. Properties of Liquids and Solutions; J.N. Murell and E. H. Boucher; John Wiley & Sons Ltd; 1982.
- 2. Principles of Colloid and Surface Chemistry; P.C. Heimenz; Marcel Dekker Inc; New York; 1986.
- 3. Surfactants and Interfacial Phenomena; M. J. Rosen; John Wiley & Sons; New York; 1989.
- 4. Colloid and Interface Chemistry; R. D. Vold and M. J. Vold; Addison-Wesley; 1982.
- 5. Surfaces, Interfaces and Colloid; D. Y. Meyer; VCH Publishers; Inc; 1991.
- 6. Surfactants and polymers in aqueous solution; Jonsson, Lindmann, Homberg and Kronberg; John Wiley and sons; 1998.
- 7. Advances in Colloid and Polymer Science; B.K.Paul&S.P.Moulik, Current Science, Vol.80, p 990-,2001; Vol.78, p 99,1998.
- 8. Critical Reviews in Food Science and Nutrition; John Flanagan & Harjinder Singh, ,Vol. 46, pp221-237, 2006.
- 9. Drug Delivery Reviews; M. J. Lawrence &G.D.Rees; Vol, 45, p 898,

#### (16 contact hours)



## Course No: CH24001OE Title: Chemistry in Everyday Life (02 Credits)

**Continuous Assessment: 10 marks** 

**Duration: 32 Contact hours End Term Exam: 40 Marks** 

**Course outcomes:** On completion of the course, the students will acquire knowledge of:

- > Chemistry involved in Water & its different methods of treatment.
- > Different household chemicals like Soaps, Detergents, Optical Brighteners, Shampoos etc.
- > Different types of Polymers used in day-to-day life.
- Chemistry of Oils and Gases.

#### UNIT-I

Max. Marks: 50

(16 contact hours)

#### Water- an amazing chemical stuff

Molecular structure and its unique properties. Composition of natural water. Hard and Soft water. Standards for drinking water. Major causes of water pollution. Methods of treatment of water for domestic purposes including Reverse Osmosis. (8 hrs)

#### **Household Chemicals**

Chemistry of soaps, detergents, optical brighteners and bleaching agents, shampoos, conditioners, dyes, hair curling and permanents, deodorants and antiperspirants, perfumes, tooth pastes and sunscreen lotions. disinfectants and moth repellents. (8 hrs)

#### Unit-II:

(16 contact hours)

#### **Polymers and Plastics:**

Characteristics and Types of Polymers. The big six of Polymer: Low Density Polyethylene (LDPE), High Density Polyethylene (HDPE), Polypropylene PP), Polystyrene (PS), Polyvinyl Chloride (PVC) and Polyethylene - Tetra phthalate (PET or PETE)- their chemical characteristics and uses. (8 hrs)

#### Oil & Natural Gases

Composition & chemical structures of petroleum products, refining of petroleum, cracking & catalytic reforming. octane & cetane rating of fuels. diesel engine fuel, kerosene and gasoline. lead in petrol: its role, disadvantages & alternatives. lpg & cng as fuel. addition of mercaptanes to natural gases for safety reasons. (8 hrs)

## **Books Recommended**

- 1. Principles of Modern Chemistry; 2nd edn; Oxtoby and Nachtrieb; Saunders College Publications; 1987.
- 2. Chemistry Fundamentals An Environmental Prospective; 2nd edn; Buell and Girad; Jones and Barlett; 2013.
- 3. www.chemistryincontext; (American Chemical Society)