

**NOORUL ISLAM CENTRE FOR HIGHER EDUCATION**  
**NOORUL ISLAM UNIVERSITY, KUMARACOIL**  
**M.Sc. CHEMISTRY**  
**CURRICULUM & SYLLABUS**  
**SEMESTER – I**

<b>SL. NO.</b>	<b>SUBJECT CODE</b>	<b>SUBJECT</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>THEORY</b>						
1.	CH1701	Organic Chemistry I	4	1	0	5
2.	CH1702	Inorganic Chemistry I	4	1	0	5
3.	CH1703	Physical Chemistry I	4	1	0	5
4.	CH1704	Basic principle of Instrumental Techniques	4	1	0	5
<b>PRACTICAL</b>						
5.	CH1771	Organic Chemistry Lab	0	0	6	6
<b>TOTAL CREDITS</b>			<b>16</b>	<b>4</b>	<b>6</b>	<b>26</b>

**Unit-I** **9**

**Chemical bonding and structure:** inductive effect - mesomeric effect - steric inhibition of resonance - ' $p\pi-d\pi$ ' bonding - hyperconjugation - cross-conjugation - hydrogen bonding - acidity, basicity, factors affecting the strength of acids and bases

**Unit-II: Introduction to Reaction Mechanism:** **9**

Kinetic and thermodynamic requirements. kinetic and thermodynamic control, Hammond Postulate, microscopic reversibility, Curtin-Hammett principle, energy profile diagram, intermediates  $V_s$  transition-states, hard and soft acids and bases. The Hammett equation and linear free energy relationships – substitution and reaction constants – Taft equation

**Methods of determining reaction mechanism:** Nonkinetic methods-Identification of products, intermediates, stereochemistry, crossover experiments, nonkinetic isotopic labeling. Kinetic methods-order, molecularity, influence of ionic strength (salt effects), primary and secondary isotopic effects.

**Unit-III** **9****a) Aromaticity**

Huckel's Rule- alternant and nonalternant hydrocarbons - concept of aromaticity, homoaromaticity and antiaromaticity - systems of 2, 4, 8 and  $10-\pi$  electrons and larger cyclic  $\pi$  systems- aromaticity of azulenes, annulenes, fulvenes, tropolones, sydnones, and fullerenes( $C_{60}$  only)

**b) Reactive Intermediates:** Formation, structure, and stabilization of carbocations, carbanions, free radicals, carbenes, and nitrenes.

**UNIT-IV Addition Reactions** **9**

Electrophilic, nucleophilic and free radical additions - Orientation and stereochemistry of addition of halogens and hydrogen halides to carbon-carbon multiple bonds - hydroboration, Sharpless asymmetric epoxidation and hydroxylation - Addition to  $\alpha, \beta$  - unsaturated carbonyl compounds - Michael reaction - condensation reactions - Perkin, Knoevenagel, Stobbe, Darzens, Sandmeyer, and Ullmann reactions.

**Unit-V Stereochemistry** **9**

**Optical isomerism:** Symmetry elements and chirality, necessary and sufficient condition for chirality - concept of prochirality - enantiotropic and diastereotropic-Fischer, Sawhorse and Newmann projection formulae and their interconversions - calculations of number of stereoisomers - R, S notations- atropisomerism - molecular dissymmetry - optical activity of allenes and spiranes - Cram's rule, Prelog's rule- stereoselective and stereospecific syntheses.

**Geometrical isomerism:** E-Z nomenclature - stereoisomerism in monocyclic compounds upto 6 membered rings - decalins and decalols, perhydrophenanthrenes and perhydroanthracenes. Conformation and reactivity of six membered ring systems.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

**Books Suggested:**

1. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi, 1989.
2. Jerry March, Advanced Organic Chemistry, 4<sup>th</sup> edition, John Wiley & Sons Inc., New York, 1992.
3. S. M. Mukherji and S.P Singh, Reaction Mechanisms in Organic Chemistry, Macmillan India Ltd., New Delhi, 1997.
4. G. M. Badger Aromatic Character and Aromaticity, Cambridge, 1969.
5. V. M. Potapov, Stereochemistry, MIR Publishers, Moscow, 1979.
6. E. L. Eliel and S. H Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, Inc. 1994.
7. D. Nasipuri, Stereochemistry of Organic Compounds, Principles and Applications, New Age International (P) Ltd., New Delhi 2000(Second Edition).
8. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press Inc., New York, 2001.
9. V. K. Ahluwalia and R. K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 2002.

**CH1702****INORGANIC CHEMISTRY – I****4 1 0 5****Unit I- Chemical Bonding****9**

Nature of covalent bond: MO theory of polyatomic molecules, ionic bond and its energetics : lattice energy – Born Lande equation and Born Haber cycle-covalent character in ionic bond- Fajan's rules, partial ionic character from dipole moment and electro negativity data – Electronagative scales- VSEPR theory – the concept of multicentre bond and structure as applied to boron hydrides.

**Unit II: Non aqueous solvents and electrode potentials****9**

General properties and classification of solvents. Self ionization and leveling effect. Reactions in non aqueous solvents- solute- solvent interation. Liquid NH<sub>3</sub>, Liquid SO<sub>2</sub>, Liquid HF.

Applications of redox potentials to Inorganic reactions – Factors affecting redox potentials.

**Unit III- Solid state chemistry****9**

Crystal defects: point, line and plane defects-intrinsic point defects: Schottky and Frenkel defects- extrinsic point defects: non-stoichiometric defect- preparation and physical properties of non–stoichiometric compounds, colour center.

Electronic structure of solids: free electron and band theories – types of solids: insulators, intrinsic and extrinsic semiconductors – optical and electrical properties of semiconductors: photovoltaic and Hall effects; p-n and n-p-n junctions and their applications as rectifier and transistor.

Superconductor, high T<sub>c</sub> superconductors-properties and applications, BCS Theory.

#### **Unit IV- Nuclear Chemistry**

**9**

Radioactive decay and equilibrium, nuclear structure and models; types of nuclear reactions- Q value, cross section - fission and fusion ; fission products and fission yields, nuclear reactors, nuclear power projects in India - radioactive techniques (radiometric titrations, isotope dilution method and neutron activation analysis), counting techniques(G.M., ionization, scintillation and proportional counters).

#### **Unit V: Lanthanides and Actinides**

**9**

Correlation of electronic structures, occurrences and properties of the elements- Chemistry of separation of Np, Pu and Am from U & fission products-Common and uncommon oxidation states-Comparison with transition elements-Lanthanide and Actinide contraction-Spectral and magnetic characteristics of Lanthanides and Actinides-Similarities between Lanthanides and Actinides-coordination compounds of lanthanides-use of lanthanide complexes as shift reagents.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

#### **REFERENCES**

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, Inorganic chemistry: principles Structure and Reactivity, 4th Ed., Harper College Publishers, 1993.
2. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo and Manfred Bochman, Advanced Inorganic Chemistry, Wiley Interscience Publication, 6th Ed., 1999.
3. G.S. Manku, Theoretical Principles of Inorganic chemistry, Tata McGraw Hill, 12th reprint, 2004.
4. K.F. Purcell and J.C. Kotz, Advanced Inorganic Chemistry, Saunders Golden Publishers.
5. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley and Sons Ltd. 2nd Ed., 1983.
6. M.c. Day Jr and J. Selbin., Theoretical Inorganic Chemistry, 2nd Ed., East West Press, 2000.
7. J.D. Lee, Concise Inorganic Chemistry, ELBS, 2006.
8. A. R. West, Solid State Chemistry and its Application, John Wiley & Sons, (Asia), 1998.
9. T. Kutty, J. Tareen, Fundamentals of Crystal Chemistry, University Press, 1st Ed., 2001.
10. L.V. Azaroff, Introduction to Solids, Tata McGraw Hill Publishing Ltd., India, 1989.
11. C. Kittel, Introduction to Solid State Physics, Wiley Eastern Ltd., 5th Ed., 1993.
12. H.V. Keer, Principles of the Solid State, Wiley Eastern Ltd., 1993.
13. D.K. Chakrabarthy, Solid State Chemistry, New Age International.
14. A.F. Wells, Structural Inorganic Chemistry, Oxford Science Publication, London, 1979.
15. M.T. Weller, Inorganic Materials Chemistry, Oxford University Press, Reprint 1996.
16. B. Sahoo, N. C. Nayak, A. Samantaray, P.K. Pujapanda, Inorganic Chemistry, PHI Learning, New Delhi, 2012.
17. Structural Principles of Inorganic Chemistry-Addison
18. Inorganic Chemistry-Gilreath

**UNIT – I: Electrochemistry I****9**

Debye- Hocket Onasger equation- derivation and experimental verification. Debye-Falkenhagen and Wein effect; activity and activity co-efficient- Debye Huckel Limiting law- derivation and verification- activity at appreciable concentration and extension of Debye Huckel theory.

Electrodics – types of electrodes- emf and its measurements- application of EMF measurements- determination of thermodynamics parameters, equilibrium constant, solubility product and dissociation constant.

**UNIT – II: Electrochemistry II****9**

Kinetics of electrode process- butler volmer equation- tafel equation-electrical double layer- zetapotential- electrokinetic phenom- over voltage- hydrogen over voltage theories of over voltage; polarography- principle and application; primary and secondary coulometer titration.

Passivity-electrochemical, chemical and mechanical passivity; corrosion- theories methods of preventing corrosion; electrochemical processes as sources of energy- dry cells storage batteries- fuel cells.

**Unit III: Chemical Kinetics-1****9**

Absolute reaction rate theory (ARRT) including thermodynamic treatment- application of ARRT to simple bimolecular processes- potential energy surfaces- kinetic isotope effect- termolecular reactions: theory of unimolecular reactions- Lindemann's theory, Hindshelwood theory, KRR theory, KRRM theory and Slater's theory .

**Unit IV: Chemical Kinetics-II****9**

Chain reactions- general characteristics- Kinetic- thermal reaction between  $H_2$  and  $Br_2$  thermal decomposition of  $N_2O_5$ , formation and decomposition of phosgene- Rice-Hertzfielmechanisims- application to reactions of 0.5, 1 and 1.5 order: explosions- Hydrogen- Oxygen reaction.

Kinetics of reactions in solution- ion- ion and ion-dipole reaction- role of dielectric constant, effect of ionic strength and influence of pressure on the reaction rates.

**Unit V: Chemical Kinetics-III****9**

Homogeneous catalysis-acid-base catalysis- methods for investigating acid base catalysis- salt effect in acid base catalysis- mechanisms of acid-base catalysis; acidity functions and their importance; Bronsted catalysis law.

Enzyme Kinetics- effect of substrate concentration- Michaelis- Menten law- Lineweaver- Burk and Eadie methods- effect of pH and temperature; inhibition competitive, uncompetitive and non-competitive inhibitions.

**L: 45 + T: 15, TOTAL: 60 PERIODS****REFERENCE**

1. K. J. Laidler, Chemical kinetics, 2<sup>nd</sup> Edition, Tata McGRaw- Hill, New Delhi, 1991.

2. K. J. Laidler, Theories of Chemical Reaction Rates, McGraw- Hill, New Delhi, 1969.
3. D. V. Roberts , Enzyme kinetics, Cambridge University Press, Cambridge, 1977.
4. J. C. Kuriacose, Catalysis, Macmillan Indian Ltd., New Delhi 1991.
5. W. J. Moore, Basic physical chemistry, Prentice Hall, 1986.
6. S. Glasstone, An introduction to electrochemistry, Van Nostrand, New York 1965.
7. J. D. M. Bockris, A. K. N. Reddy, Modern Electrochemistry, Vol. I & II, Plenum Press, New York, 3<sup>rd</sup> Reprint, 1977.
8. J. Bard, L. R. Faulkner, Electrochemical Methods: Fundamentals and Application. John Wiley and Sons, New York, 1980.
9. D. R. Crow, Principles and applications of Electrochemistry, Chapman and hall, London 1979.

## **CH1704 BASIC PRINCIPLE OF INSTRUMENTAL TECHNIQUES 4 1 0 5**

### **Unit I - UV - Visible and IR spectroscopy 9**

UV - Visible spectroscopy: Various electronic State - Beer lambert law - effect of solvent on electronic transitions.

IR spectroscopy: Requirements for IR absorption - Instrumentation and sample handling - different types of stretching and bending vibrations - far IR region.

### **Unit II: NMR and ESR spectroscopy 9**

Nuclear Magnetic Resonance spectroscopy: Origin - Shielding and deshielding mechanism -chemical shift - spin -spin interaction - coupling constant.

Electron Spin Resonance spectroscopy: Theory of ESR - comparison between ESR and NMR - hyperfine coupling.

### **Unit III: Mass Spectrometry and TGA/DTA 9**

Mass Spectrometry: Ionization sources - simple instrumentation techniques - molecular ions -metastable ions.

TGA/DTA: Differential thermal analysis (DTA) - Differential scanning calorimetry (DSC) - Thermogravimetric analysis (TGA) - methodology of TGA/DTA.

### **Unit IV: Ramam and Mossbauer Spectroscopy 9**

Raman Spectroscopy: Theory - sample handling - comparison of Raman and IR Spectroscopy.

Mossbauer Spectroscopy: Basic principles - spectral parameters and spectrum display detection of oxidation states.

### **Unit V: X-ray diffraction and Neutron diffraction 9**

X -ray diffraction: Bragg condition - Miller indices - Laue method - Bragg method - different types of unit cells - single crystal and powder XRD methods.

Neutron diffraction: Scattering of neutrons by solids and liquids - Magnetic scattering.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

### **Books suggested**

1. H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, Instrumental methods of Analysis, 7<sup>th</sup> EDN, CBS Publishers, 1986.
2. R. West, Solid state chemistry and its application, wiley, Reprint 2004.

### **CH1771**

### **ORGANIC CHEMISTRY LAB 0 0 6 6**

1. Double stage preparations involving reactions such as bromination, nitration, oxidation, reduction, hydrolysis, diazotization, acetylation *etc.*
2. IR spectra of the synthesized components recorded (demonstration only).
3. Estimation of phenol, aniline, methyl ethyl ketone, glucose (both Bertrand's and Lane and Eynone methods).
4. Extraction of caffeine from tea leaves, piperine from black pepper, lycopene from tomatoes, limonene from orange peels, ascorbic acid from lemon or gooseberry, eugenol from cloves (demonstration only).
5. Determination of R<sub>f</sub> values by thin layer chromatography (TLC) (demonstration only).
6. Estimation of amino acids, nitro group, carboxylic acid, formalin, and acetyl group (for class work only)  
  
Micro methods may be used wherever possible.

### **Books Suggested:**

1. Experimental Organic Chemistry – M. P. Doyle and W. S. Mungall.
2. A Text Book of Practical Organic Chemistry – A. I. Vogel.
3. Techniques and Experiments for Organic Chemistry – Addison Ault.
4. Advanced Practical Organic Chemistry – N. K. Vishnoi.
5. Laboratory Manual of Organic Chemistry – B. B. Dey and M. V. Sitaraman.
6. Laboratory Manual in Organic Chemistry – R. K. Bansal.

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**M.Sc. CHEMISTRY**  
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**SEMESTER – II**

<b>SL. NO.</b>	<b>SUBJECT CODE</b>	<b>SUBJECT</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>THEORY</b>						
1.	CH1705	Organic Chemistry II	4	1	0	5
2.	CH1706	Inorganic Chemistry II	4	1	0	5
3.	CH1707	Physical Chemistry II	4	1	0	5
4.	Xxx2	(Supportive course paper - I)	4	0	0	4
<b>PRACTICAL</b>						
5.	CH1772	Inorganic Chemistry Lab	0	0	6	6
<b>TOTAL CREDITS</b>			<b>16</b>	<b>3</b>	<b>6</b>	<b>25</b>



**Unit-I****9****a) Aliphatic Nucleophilic Substitution**

$S_N1$ ,  $S_N2$ ,  $S_{Ni}$ ,  $S_{Ni}'$  and tetrahedral mechanisms - ambident nucleophiles and ambident substrates - effect of substrate, attacking nucleophile, leaving group, and reaction medium - neighbouring group participation (NGP), anchimeric assistance.

**b) Aromatic Nucleophilic Substitution:**

$S_{NAr}$ ,  $S_{N1}$ , and benzyne mechanisms - structure-reactivity relationship-Ziegler alkylation and Chichibabin reaction, Rosenmund reaction, von Braun reaction.

**Unit-II****9****a) Aliphatic Electrophilic Substitution:**

Bimolecular mechanisms-  $S_E2$  and  $S_{Ei}$ . The  $S_{E1}$  mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. Stork enamine reaction.

**b) Aromatic Electrophilic Substitution Reactions:**

Arenium ion and  $S_{E1}$  mechanisms. Orientation and reactivity of monosubstituted benzene rings - ortho/para ratio - Ipso attack. Quantitative treatment of reactivity in the substrates and electrophiles, diazonium coupling effect of leaving group, formylation - Gattermann, Gattermann-Koch reactions - Reimer-Tiemann, Kolbes, Vilsmeier-Haak, Bischler-Napieralski, Hofmann - Martius and Jacobson's reactions, Friedel-Crafts alkylation and acylation.

**Unit-III Heterocycles****9**

General methods of synthesis and reactions of carbazoles, acridines, imidazoles and pyrazoles, oxazoles and isoxazoles, thiazoles and isothiazoles, pyridazine, pyrimidine and pyrazines,  $\alpha$ - and  $\gamma$ -pyrones, benzotriazole. Synthesis and applications of polypyrrole and polythiophene.

**UNIT-IV Elimination Reactions****9**

The  $E1$ ,  $E2$ ,  $E1cB$  mechanisms - stereochemistry of eliminations - elimination versus substitution - orientation of double bond - Saytzeff and Hoffman rules - pyrolytic eliminations - mechanism of pyrolysis of esters of carboxylic acids -Chugaev reaction - Hofmann degradation - Cope elimination.

**UNIT-V Alkaloids and Terpenoids:****9**

Alkaloids: Classification – General methods of determining the structure – structural elucidation, synthesis and stereochemistry of morphine, reserpine, and quinine – Biosynthesis of alkaloids.

Terpenoids: Structural elucidation, synthesis and stereochemistry of camphor, zingiberene, santonin, and abietic acid – Biosynthesis of terpenoids.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

**Books Suggested:**

1. Peter Sykes, A Guidebook to Mechanism in Organic Chemistry, Orient Longman, New Delhi, 1989.
2. Jerry March, Advanced Organic Chemistry, 4<sup>th</sup> edition, John Wiley & Sons Inc., New York, 1992.
3. S. M. Mukherji and S.P Singh, Reaction Mechanisms in Organic Chemistry, Macmillan India Ltd., New Delhi, 1997.
4. R. K. Bansal, Heterocyclic Chemistry, Wiley Eastern Ltd., New Delhi, 1990.
5. R. M. Acheson, An Introduction to the Chemistry of Heterocyclic Compounds, Wiley Eastern Ltd., New Delhi.
6. I. L. Finar, Vols. I and II

**CH1706****INORGANIC CHEMISTRY – II****4 1 0 5****Unit-I- Coordination Chemistry I****9**

VB,CF and MO theories of complexes with four and six coordination numbers- CFSE-factors affecting the magnitude of  $10 Dq$  values –spectrochemical series- applications of CFT – site preferences in spinels- nephelauxetic effect- bonding and MO theory – static and dynamic John-Teller behavior.

**Unit-II- Coordination Chemistry II****9**

Thermodynamic stability – stepwise and overall stability constants and their relationship – determination of stability constant by potentiometric and spectrophotometric methods, factors affecting stability: chelate effect, kinetic and thermodynamic template effects and their application in the synthesis of macrocyclic ligands; HSAB Concept: applications and theoretical basis, characterization of stabilities of mixed ligand complexes.

**Unit-III- Coordination Chemistry III****9**

Kinetic stability, lability and inertness; ligand substitution reactions in octahedral and square planar complexes : acid hydrolysis, base hydrolysis and anation reactions; trans effect – theories and applications; electron transfer reactions : complementary and non-complementary types; inner and outer-sphere processes – applications of electron transfer reactions in synthesis of coordination complexes – reactions of coordinated ligand : mechanism of ascorbic acid oxidation by free and chelate Cu(II) Complexes.

**Unit – IV: ORGANOMETALLIC CHEMISTRY – I****9**

Introduction - History-EAN and its correlation to stability- Synthesis and structures of metal carbonyls- carbonylate anions, carbonyl hydride complexes and metal nitrosyls-IR study of metal carbonyls-Synthesis, properties and structural features of metal complexes with carbene, alkene, alkyne and arene. Hapticity-Metallocenes-synthesis, properties and bonding in ferrocene-covalent versus ionic bonding in beryllocene, clusters and catalysis, hydride and dihydrogen complexes, fluxionality.

**Unit – V: ORGANOMETALLIC CHEMISTRY – II****9**

Oxidative addition and reductive elimination- insertion and elimination reactions nucleophilic and electrophilic attack of coordinating ligands- Catalysis by organometallic

compounds-Homogeneous catalysis-alkene hydrogenation- synthesis gas and water-gas shift reaction- hydroformylation- carbonylation of alcohols and oxygenation of olefins-Heterogeneous catalysis-Fischer-Tropsch process and Ziegler—Natta polymerization-Immobilized homogeneous catalysts.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

#### **REFERENCE**

1. James E. Huheey, Ellen A. Keiter and Richard L. Keiter, Inorganic chemistry: Principles, Structure and Reactivity, 4th Ed., Harper Collins College Publishers, 1993.
2. F. Albert Cotton, Geoffrey Wilkinson, Carlos A. Murillo and Manfred Bochman, Advanced Inorganic Chemistry, Wiley Interscience Publication, 6th Ed., 1999.
3. D. Bannerje, Coordination Chemistry, Tata McGraw Hill, 1993.
4. G.S. Manku, Theoretical Principles of Inorganic Chemistry Tata McGraw Hill, 12th reprint 2004.
5. K.F. Purcell and J.C. Kotz, Advanced Inorganic Chemistry, Saunders Golder Publishers.
6. B.E. Douglas, D.H. McDaniel and J.J. Alexander, Concepts and Models of Inorganic Chemistry, John Wiley and Sons Ltd., 2nd Ed., 1983.
7. M.C. Day Jr and J. Selbin, Theoretical Inorganic Chemistry, 2nd Ed., East West Press, 2000.
8. J.D. Lee, Concise Inorganic Chemistry, ELBS, 2006.
9. D.F. Shriver, P.W. Atkins and C.H. Langford, Inorganic Chemistry, ELBS, Oxford University Press, 1994.
10. W.L. Jolly, Modern Inorganic Chemistry, McGraw Hill Company, 2nd Ed., 1991.
11. R.S. Drago, Physical Methods in Inorganic Chemistry, Saunders College Publishers.
12. E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, Structural Methods in Inorganic Chemistry, ELBS, 1988.
13. D.A. Skoog, F. James Holler and J.A. Nieman, Principles of Instrumental Analysis, Saunders, 1992.
14. H.H. Willard, L.L. Merritt and J.A. Dean, Instrumental Methods of Analysis, CBS Publishers, 6th edition, 1986.
15. G.H. Jeffery et al., Vogel's Textbook of Quantitative Chemical Analysis, Revised 5th edition, ELBS, 1989.
16. R.A. Day and A.L. Underwood, Quantitative Analysis, Prentice Hall, 1999.
17. Coordination Chemistry- Kettle.
18. Reaction mechanism- Basalo and Pearson
19. Coordination Chemistry- Basalo and Johnson
20. Inorganic Chemistry- P. B. Janadhanam shivashankar.

**Unit I- Quantum Chemistry-I****9**

Planck's Quantum theory- Wave particle duality – uncertainty principle, operators and commutation relation, postulates of quantum mechanics – simple system – one dimensional box, three dimensional box – rigid rotator – harmonic oscillator – hydrogen atom.

**Unit –II- Quantum Chemistry-II****9**

Many electron system – Pauli antisymmetry principle – Slater determinant – Approximation methods – variation and perturbation – application to helium atom – Hartree Self Consistent field theory.

Born – Oppenheimer approximation – LCAO – MO for  $H_2^+$  ion – VB treatment of  $H_2$  molecule. Hybridisation –  $sp$ ,  $sp^2$ ,  $sp^3$ , HMO theory – ethylene and butadiene.

**Unit –III- Thermodynamics-I****9**

Thermodynamics of system of variable composition – partial molar properties – chemical potential – Gibbs Duhem equation – apparent molar properties – methods of determination of partial molar quantities, partial molar thermal properties – differential and integral heats of solution.

Thermodynamic properties of real gases – fugacity concept – determination of fugacity – real and mixture of gases – Lewis – Randall rule. Nernst heat theorem – different forms of stating the third law – thermodynamic quantities at absolute zero.

**Unit-IV- Thermodynamics-II****9**

Ensemble of systems – state of a system – phase space – statistical equilibrium – microcanonical and grand canonical ensemble – micro and macro states; derivation of classical Boltzmann distribution law; quantum statistics – Bose – Einstein, Fermi- Dirac and Maxwell-Boltzmann statistics – comparison of B.E and F.D statistics with Boltzmann statistics – photon gas and electron gas; Boltzmann-Planck equation; partition function – partition function and thermodynamic properties – partition function and equilibrium constant; concept of negative Kelvin temperature.

**Unit V: Photochemistry****9**

Photophysical process in electronically excited molecules – fluorescence, phosphorescence delayed emission and other deactivation processes – Stern- Volmer equation and its application, photosensitization – chemiluminescence; conventional photolysis procedure – flash photolysis; elementary aspects of photosynthesis; photochemical chain reactions H-Br reaction – ozone depletion – photochemical conversion and storage of solar energy.

**L: 45 + T: 15, TOTAL: 60 PERIODS****REFERENCES:**

1. A.K. Chandra, Introduction to quantum Chemistry, Tata McGraw Hill, New Delhi, 1997.
2. L.N. Levine, Quantum Chemistry, Prentice Hall, New Delhi 1994.

3. R.K. Prasad Quantum Chemistry, Wiley Eastern, 1993.
4. F.E. Pilar, Elementary Quantum Chemistry, McGraw Hill, New Delhi, 1968.
5. S. Glasstone, Theoretical Chemistry, Van Nostrand, New York, 1944.
6. S. Glasstone, Thermodynamics for chemists, Van Nostrand, New York, 1969.
7. M.C. Gupta, Statistical Thermodynamics, Wiley-Eastern, New Delhi, 1990
8. J.Rajaram, J.C. Kuriaacose, Thermodynamics for chemistry, Shoban Lal Nagain Chand, New Delhi, 1986.
9. K.K. Rohatgi- Mukerkkjee, Fundamentals of Photochemistry, Wiley-Eastern, New Delhi, 1978.
10. J.R. Lakowicz, Principls of Fluoresence Spectroscopy, Plenum Press, New York, 1999.
11. N.J. Turro, Molecular Photochemistry, Benjamin, 1965.
12. J.G. Calvert, J.N. Pitts, Photochemistry, Wiley, New York, 1966.

**CH1772**

**INORGANIC CHEMISTRY LAB**

**0 0 6 6**

1. Semi micro qualitative analysis of inorganic mixture containing two less familiar cations  
  
W, Tl, Se, Mo, Ce, Th, Zr, Ti, V, U and Li
2. Complexometric titrations – Estimation of Cu, Zn and Mg by EDTA titration in the presence of either Pb or Ba
3. Preparation of coordination complexes

**Reference**

1. V.V.Ramanujam, 'Inorganic semimicro Qualitative analysis, 3<sup>rd</sup> revised Edn, National Publishing Co., Chennai, 1988.

Vogel's Text book of Qualitative chemical analysis, Eds. G.H.Jeffrey, J.Banett, J.Mendham and R.C.Denney, ELBS, 5<sup>th</sup> Edn, 1991.

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**SEMESTER – III**

<b>SL. NO.</b>	<b>SUBJECT CODE</b>	<b>SUBJECT</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
<b>THEORY</b>						
1.	CH1709	Organic Chemistry III	4	1	0	5
2.	CH1710	Inorganic Chemistry III	4	1	0	5
3.	CH1711	Physical Chemistry III	4	1	0	5
4.	Xxx2	(Supportive course paper - II)	4	0	0	4
<b>PRACTICAL</b>						
5.	CH1773	Physical Chemistry Lab	0	0	12	6
<b>TOTAL CREDITS</b>			<b>16</b>	<b>3</b>	<b>12</b>	<b>25</b>

**Unit I:****9****a) UV Spectroscopy**

Various electronic transitions (185–800 nm), Beer–Lamberts law, effect of solvent on electronic transitions, ultraviolet bands for saturated and unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser–Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds – Scott's rules – shift reagents – steric effect in biphenyls.

**b) IR Spectroscopy**

Instrumentation and sample handling – characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams, and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FT–IR.

**c) ORD and CD**

Definition, -haloketo rule, deduction of absolute configuration, Octant rule for ketones – Applications of ORD and CD

**Unit II:****9****a) <sup>1</sup>H–NMR Spectroscopy**

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon–(aliphatic, olefinic, acetylenic, aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides and mercaptans), chemical exchange, effect of deuteration, complex spin–spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve – variation of coupling constant with dihedral angle. Simplification of complex spectra – double resonance, shift reagents, NOE, FT–technique – Spin Relaxation.

**b) C–NMR Spectroscopy**

General considerations – chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. 2-D NMR–COSY, DEPT, Magnetic Resonance Imaging (MRI)

**Unit III:****9****a) Mass spectrometry**

Introduction to EI. Factors affecting fragmentation. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, nitrogen rule, metastable peak, McLafferty rearrangement – Isotopic peaks, CI, FAB, MALDI.

**b) Combined Spectral Problems:**

Spectral problems involving UV, IR, NMR and Mass spectral data.

**Unit IV:****9****a) Selected Name Reactions:**

Aldol, Dieckmann condensations–Reformatsky, Grignard, Wittig and Mannich reactions–Robinson annulation–Oppenauer oxidation – Clemmenson, Wolff-Kishner, Meerwin-Pondorf-Verley (MPV) and Birch reductions–Nef reaction, McMurry reaction, Japp-Klingemann reaction, Polonovski reaction.

**b) Retro-Synthetic Analysis:**

Strategy and planning–starting material–Linear and Convergent approach, protecting groups and activating groups. regio-selectivity, chemoselectivity. diastereoselectivity. Target molecule containing one functional group requiring a single disconnection–Synthons and synthetic equivalents. Latent polarity. Target molecules with two functional groups– 1, 2-, 1, 3- 1, 4-, 1, 5-, and 1, 6-dicarbonyl compounds, Umpolung. Functional group interconversions (FGI).

**Unit V:****9****Supra molecular Chemistry:**

Definition – host-guest chemistry – classification of supramolecular host-guest compounds – coordination and the lock and key analysis – the chelate, macrocyclic and template effects – nature of supramolecular interactions – spherands, lariat ethers, podants, cryptands – molecular recognition, chiral recognition, molecular sieves, molecular wires, molecular switches.

**L: 45 + T: 15 = TOTAL: 60 PERIODS****REFERENCES**

1. R.M. Silverstein, G.C. Bassler, T.C. Morrill, Spectrometric Identification of Organic Compounds, John Wiley & Sons, New York, 1991.
2. W. Kemp, Organic Spectroscopy, Macmillan Press Ltd. 1996.
3. D.H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill, New Delhi, 1988(Fourth Edition)
4. Jag Mohan, Organic Spectroscopy, Principles and Applications, Narosa publishing House, New Delhi, 2001.
5. P.Y. Bruice, Organic Chemistry, Pearson Education, Inc., Delhi, 2002.
6. P.R. Young, Practical Spectroscopy, The Rapid Interpretation of Spectral Data Brooks/Cole, California, 2000.
7. R. Davis, M. Frearson, Mass Spectrometry, John Wiley & Sons, New York, 1991
8. S. Warren, Designing Organic Syntheses: A Programmed Introduction to the Syntheses Approach, John Wiley & Sons, 1978.
9. C.L Willis and M Wills, Organic Syntheses, Oxford University Press, 1995.
10. R.E. Ireland, Organic Synthesis, Prentice-Hall of India Pvt. Ltd, New Delhi, 1975.
11. J.W. Steed and J.L. Atwood, Supramolecular Chemistry, John Wiley & Sons, New York.



**Unit I: Group Theory-I**

9

Symmetry properties of molecules and group theory

Symmetry elements, symmetry operations and point groups, properties of groups, symmetry and dipole moment, symmetry and optical activity, symmetry operations as a group, multiplication table. Classes of symmetry operations, matrix representation of operations - Reducible and irreducible representation, orthogonality theorem. Properties of irreducible representations. Construction of character table for point groups ( $C_{2v}$ ,  $C_{3v}$ ,  $C_{2h}$ ,  $C_{4v}$  and  $D_2$ ). Explanations for the complete table for a point group.

**Unit II: Group Theory-II**

9

Application of group theory:

Symmetry selection rules for IR, Raman and electronic spectra

Symmetry reduction formula. Determination of representations of vibrational modes in non-linear molecules ( $H_2O$ ,  $NH_3$  and Trans  $N_2F_2$ ). Infra red and Raman activities of normal modes of vibrations. Rule of mutual exclusion.

Electronic spectra of ethylene and formaldehyde molecules. Hybrid orbital in non-linear molecules ( $CH_4$ ,  $XeF_4$ ,  $BF_3$  and  $PF_3$ ). Projection operators and symmetry adapted linear combinations(SALC). Simplifications of HMO calculations using group theory.

**Unit-III**

9

**Application of spectroscopy to the study of Inorganic compounds - I**

**NMR spectroscopy:**  $^{31}P$ ,  $^{19}F$  and  $^{15}N$ -NMR – Introduction, applications of structural problems-evaluation of rate constants-monitoring the course of reaction-NMR of fluxional molecules – NMR of paramagnetic molecules-contact shifts and shift reagents.

**ESR spectroscopy:** Principles – preparation of the spectrum – hyperfine splitting – factors affecting the magnitude of g-values-zero field splitting and Kramer's degeneracy-anisotropy in the hyperfine coupling constant. Application of ESR in the study of transition metal complexes – J-T-distortion: studies of Cu(II) complexes.

**Unit-IV**

9

**Application of spectroscopy to the study of Inorganic compounds - II**

Applications of IR and Raman spectra in the study of coordination compounds: Application to metal carbonyls and nitrosoyls – geometrical and linkage isomerism – detection of inter and intramolecular hydrogen bonding – stretching mode analysis of metal carbonyls.

Mossbauer spectroscopy: Principle – application of isomer shift, quadrupole interactions and magnetic splitting in the study of iron and tin compounds.

**Unit-V**

9

**Application of spectroscopy to the study of Inorganic compounds - III**

Electronic spectroscopy – L-S coupling and j-j coupling scheme, micro states, Hund's rule and term symbols. Selection rules for electronic transition and hole formalism – splitting of terms – Orgel and Tanabe Sugano diagrams – Evaluation of  $10 Dq$  and  $B$  for

octahedral d2 and d8 systems. Charge transfer spectra. Electronic spectra of Lanthanide and actinide complexes.

Photoelectron spectroscopy: Koopman's theorem. PES – XPES (ESCA)- chemical shifts in XPS- application of ESCA to inorganic systems- Auger electron spectroscopy.

**L: 45 + T: 15 = TOTAL: 60 PERIODS**

## REFERENCES

1. F.A. Cotton, Chemical Applications of Group Theory, Wiley-Eastern, New Delhi, 1971.
2. G. Davidson, Introductory Group Theory for Chemists, Applied Science Publishers, London, 1971.
3. V. Ramakrishnan and M.S. Gopinathan, Group theory and Chemistry, Vishal Publications, Delhi, 1991.
4. K.V. Raman, Group theory and its Applications to Chemistry, Tata McGraw-Hill, New Delhi, 1990.
5. D.C. Harris, M.D. Bertolucci, Symmetry and Spectroscopy, Oxford University Press, New York, 1978.
6. R.S. Drago, Physical Methods in Chemistry, Saunders, London, 1977.
7. C.N. Banwell, Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1990.
8. R. Chang, Basic Principles of Spectroscopy, McGraw-Hill, New Delhi, 1971.
9. G.M. Barrow, Introduction to Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1964.
10. B.P. Straughan and S. Walker, Spectroscopy, Vol. 1, 2 & 3, Chapman and Hall, London, 1976.
11. A. Carrington and A.D. McLachalan, Introduction to Magnetic Resonance, Harper and Row, New York, 1976.
12. Organic Structure Determination – D.J. Pasto and ER. Johnson– Prentice-Hall, Inc., 1969.

**CH1711**

**PHYSICAL CHEMISTRY-III**

**4 1 0 5**

### **UNIT-I: Polymer Chemistry**

**9**

Natural and synthetic polymers – general concept – chemical heterogeneity-polymolecularity – radical, ionic and coordination chain polymerization; stereospecific polymerization and the utility of Ziegler-Natta catalyst; copolymerization – synthesis of graft and block copolymers; polystyrene, acrylic polymers and polyesters, cellulosic polymers, phenol resins, amino resins and epoxy resins – mechanism of radical and ionic polymerization.

Conducting polymers – chemical structure and electronic behavior of polymers – doping of conducting polymers – such as polyaniline, polypyrrole and polythiophene.

## **Unit II: Molecular Spectroscopy-I**

**9**

Characterization of electromagnetic radiation - signal to noise ratio – the width and intensity of spectral transitions; microwave spectroscopy – rotational spectra of diatomic and simple polyatomic molecules; infrared spectroscopy – harmonic and anharmonic oscillator – vibration – rotation spectra of diatomic and polyatomic molecules- influence of rotation on the spectra of polyatomic molecules – parallel and perpendicular vibrations.

Raman spectroscopy – theory of Raman effect – pure rotational Raman spectra - vibrational Raman spectra –mutual exclusion principle

## **Unit III: Molecular spectroscopy-II**

**9**

Electronic spectroscopy – Born- Oppenheimer approximation – vibrational coarse structure – Franck-Condon principle – dissociation energy – rotational fine structure of electronic – vibration transitions- Fortrat diagram – predissociation.

NMR Spectroscopy – spin and an applied field – nature of spinning particles – interaction of spin magnetic field – population of energy levels; chemical shift and coupling constant

NQR spectroscopy – principles- experimental set up- nuclear quadrupole coupling in atoms and molecules – applications; ESR spectroscopy – basis principles – hyperfine splitting – origin of hyperfine interaction – the g value – Mc Connel relationship – applications of ESR.

## **UNIT-IV: Adsorption and surface phenomenon**

**9**

Physisorption and chemisorptions, adsorption and desorption, adsorption isotherms – Langmuir and B.E.T. equation and significance in surface area determination, surface films, adsorption from solution, Gibb's adsorption equation: derivation, significance. Kinetics of unimolecular and bimolecular surface reactions. Applications of photoelectron spectroscopy, ESCA and Auger spectroscopy to the study of surfaces.

Surface activity, surface active agents and their classification, micellisation, critical micelle concentration (cmc), thermodynamics of micellisation, factors affecting cmc, methods of determination of cmc, use of surfactants in oil recovery.

## **UNIT-V: Nanomaterials**

**9**

Nanoscience: Introduction, classification of nanomaterials: definition and examples of zero, 1F, 2D and 3D Nanostructures- Properties of nanomaterials – physical properties – finite size effects – optical, magnetic and electronic properties-Turbevitch and Brust method of preparation of nanogold and other noble metals- surface plasma resonance of nanogold and its applications in sensors.

**L: 45 + T: 15 = TOTAL: 60 PERIODS**

## **REFERENCES**

1. F. A. Cotton, Chemical Applications of Group Theory, Wiley-Eastern, New Delhi, 1971.
2. G. Davidson, Introductory Group Theory for Chemists, Applied Science Publishers, London, 1971.

3. V. Ramakrishnan and M. S. Gopinathan, Group theory and Chemistry, Vishal Publications, Delhi, 1991.
4. K.V. Raman, Group theory and its Applications to Chemistry, Tata McGraw-Hill, New Delhi, 1990.
5. D. C. Harris, M.D. Bertolucci, Symmetry and Spectroscopy, Oxford University Press, New York, 1978.
6. R. S. Drago, Physical Methods in Chemistry, Saunders, London, 1977.
7. C.N. Banwell, Fundamentals of Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1990.
8. R. Chang, Basic Principles of Spectroscopy, McGraw-Hill, New Delhi, 1971.
9. G. M. Barrow, Introduction to Molecular Spectroscopy, Tata McGraw-Hill, New Delhi, 1964.
10. B.P. Straughan and S. Walker, Spectroscopy, Vol. 1, 2 & 3, Chapman and Hall, London, 1976.
11. C. D. Becker, High Resolution NMR – Theory and Applications, Academic Press, New York, 1980.
12. D. W. Claridge, High Resolution NMR Techniques in Organic Chemistry, Pergamon, 1999.
13. F. W. Billmeyer, Jr., Text Book of Polymer Science, 3<sup>rd</sup> Edition, John Wiley and Sons, New York, 1984.
14. A. Tager, Physical Chemistry of Polymers, Mir Publishers, Moscow, 1978.
15. F. Rodriguez, Principles of Polymer Systems, 2<sup>nd</sup> Edition, McGraw-Hill, New Delhi, 1987.
16. V. R. Gowariker, N.V.Viswanathan and J. Sreedhar, Polymer Science, Wiley-Eastern, New Delhi 1988.
17. B. Bahadur and N.V.Sastry, Principles of Polymer Science, Narosa, New Delhi, 2002
18. J. E. Katon, Organic Semiconducting Polymers, Marcel Dekker, New York, 1968.

**CH1773**

**PHYSICAL CHEMISTRY LAB**

**0 0 12 6**

1. Adsorption

Adsorption of acetic acid/ oxalic acid on activated charcoal- Verification of Freundlich isotherm- determination of unknown concentration

2. Potentiometric titration

(i) Redox

FAS vs  $\text{Ce}^{4+}$

$\text{Fe}^{2+}$  -  $\text{KMnO}_4$

KI -  $\text{KMnO}_4$

(ii) Precipitation

$\text{KCl}$  -  $\text{AgNO}_3$

$\text{KCl}$  + KI -  $\text{AgNO}_3$

3. Conductivity

Determination of solubility product of a sparingly soluble salt

Titration (mixture of acids vs NaOH)

4. Thermometry

Determination of solution enthalpy

(i) Oxalic acid – water

(ii) Ammonium oxalate – water

5. Distribution

Distribution of benzoic acid between benzene /toluene & water

**NOORUL ISLAM CENTRE FOR HIGHER EDUCATION**  
**NOORUL ISLAM UNIVERSITY, KUMARACOIL**  
**M.Sc. CHEMISTRY**  
**CURRICULUM & SYLLABUS**  
**SEMESTER – IV**

<b>SL. No.</b>	<b>Course Code</b>	<b>Course Title</b>	<b>L</b>	<b>T</b>	<b>P</b>	<b>C</b>
1.	Xx17E1	Elective - I	4	0	0	4
2.	Xx17E2	Elective - II	4	0	0	4
<b>PRACTICAL</b>						
3.	CH17P1	Project and Viva - Voce	0	0	12	6
<b>TOTAL</b>			<b>8</b>	<b>0</b>	<b>12</b>	<b>14</b>

**NOORUL ISLAM CENTRE FOR HIGHER EDUCATION**

**NOORUL ISLAM UNIVERSITY, KUMARACOIL**

**M.Sc. CHEMISTRY**

**LIST OF ELECTIVES**

<b>LIST OF SUPPORTIVE COURSES</b>						
1.	PH1713	Basic Biophysics	3	1	0	4
2.	PH1714	Renewable energy	3	1	0	4
3.	CH1708	Chemistry and Industry	4	0	0	4
4.	CH1712	Chemistry and Environment	4	0	0	4
<b>LIST OF ELECTIVES</b>						
1.	CH17A3	Advanced Organic Chemistry	4	1	0	5
2.	CH17A4	Inorganic Materials and Bioinorganic Chemistry	4	1	0	5
3.	CH17A5	Physical Chemistry – Catalysis	4	1	0	5

## ELECTIVE PAPER - I

PH1713

BASIC BIOPHYSICS

3 1 0 4

### UNIT I: Basics of Biophysics

9

Role of biomolecules in biological functions, Atoms bonds, types of bonds, molecular configuration and conformation, structural isomerism, geometrical isomerism, optical isomerism, optical activity, basis of molecular interactions, Lennard –Jones potential, various bonds involved in structural stabilization of biomolecules.

### UNIT II: Proteins

9

Structure and properties of amino acids, peptide unit, allows conformation for a pair of links peptide units, Ramachandran contact criteria and Ramachandran map, Primary Secondary Tertiary and Quaternary structure of proteins stabilizing forces in proteins, globular and fibrous proteins.

### UNIT III: Nucleic acids

9

Nucleotides, Double helical structure of DNA, Watson and Crick model, base pairing and base stacking, Interactions stabilizing the structure of DNA, A,B and Z forms of DNA, structure of tRNA.

### UNIT IV: Carbohydrates

9

Structure and conformations of monosaccharide's chair and boat conformations Disaccharides, glycosidic linkage and glycosidic torsional angles, conformational map for disaccharides , oligosaccharide and polysaccharide structure of cellulose and amylose glycoproteins and glycolipids.

### UNIT V: Biological Databases

9

Database in proteins, Sequence database, Structural database, sequence comparison methods Nucleic acid database, Human genome mapping project, carbohydrate database.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

### Basic for Study and References:

1. Basic Biophysics  
Vasanthi Pattabhi and N. Goutham,  
Alpha Science International,2002
2. P.Narayanan  
Essentials of Biophysics  
New Age International,2000
3. Biochemistry  
Jeremy M.Berg, John L.Tymoczko and Lubert Stryer  
W.H.Freeman 2002, 5<sup>th</sup> Edition
4. [www.3DS.DSCAR.ORG](http://www.3DS.DSCAR.ORG)
5. Conformations of Carbohydrates



R.Chandrasekarans, P.V.Balaji, P.K.Qasba and V.S.R.Rao  
Harwood Academic Press, 1998

**PH1714**

**RENEWABLE ENERGY**

**3 1 0 4**

**UNIT I: Energy**

**9**

Energy – forms of energy – measurement - non-renewable energy and renewable energy –types and sources. Energy conservation- carbon sequestration.

**UNIT II: Solar Energy and Geothermal Energy**

**9**

Solar thermal energy - various methods of using solar energy – photovoltaic cell, solar cooker and water heater - artificial photosynthesis - advantages and disadvantages of solar energy. Geothermal energy – resources - geothermal exploration - geothermal heat pump - types - geothermal desalination - advantages and disadvantages of geothermal energy.

**UNIT III: Wind Energy and Wave Energy**

**9**

Wind energy – wind turbine – types - factors affecting efficiency of wind turbines – wind farm – capacity factor- factors affecting. Wave energy - wave motion– wave power formula, wave energy and energy flux. Ocean Thermal Energy Conversion (OTEC) – ocean wave energy devices -OTEC power generation.

**UNIT IV: Hydro Energy and Biomass**

**9**

Hydropower –generation methods - types of turbine - power calculation - advantages and disadvantages. Biomass – conversion process – types - biomass for power and heat – biofuels – types of biofuels - advantages and disadvantages.

**UNIT V: Hydrogen Energy and Fuel Cell**

**9**

Hydrogen as a renewable energy source - sources of hydrogen - hydrogen production - direct electrolysis of water - thermal decomposition of water - biological and biochemical methods. Storage of hydrogen. Fuel cell – working principle – Types of fuel cells and applications. advantages and disadvantages of fuel cells.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

**Reference Books:**

1. G. N. Tiwari, Rajeev Kumar Mishra. Advanced Renewable Energy Sources. Royal Society of Chemistry, 2011
2. D. Mukherjee. Fundamentals of Renewable Energy Systems. New Age International, 2007
3. S. A. Abbasi, Naseema Abbasi. Renewable Energy Sources and Their Environmental Impact. PHI Learning Pvt. Ltd., 2004
4. S. L. Sah. Renewable and Novel Energy Sources. M.D. Publications Pvt. Ltd., 1995
5. Paul Komor. Renewable Energy Policy. iUniverse, 2004
6. Tushar K. Ghosh, Mark A. Prelas. Energy Resources and Systems Volume 2: (2011), springerlink

7. Dr. Sathyajith Mathew Wind Energy Fundamentals, Resource Analysis and Economics (2006), springerlink
8. S.P. Sukhatme. Solar Energy Principles of Thermal Collection and Storage, 2nd Ed. TMH
9. N.K Bansal, M. Kleemann & M. Melss, Renewable Energy Source and Conversion Technology, TMH.
10. G.T. Wrixon, A.M.E. Rooney & W. Palz, Renewable Energy. Springer Verlag 2000
11. D.O.Hall and R.P. Overeed. Biomass Renewable Energy – ( John Wiley and Sons, New york, 1987)

**CH1708**

**CHEMISTRY AND INDUSTRY**

**4 0 0 4**

**Unit-I: Petroleum Products**

**9**

Petroleum –its occurrence, mining, composition and classification; distillation of crude petroleum; gasoline for motor and aeroplanes, diesel and kerosene knocking and anti-knocking; octane number;pyrolysis of heavy oil and production of gasoline

**Unit-II: Plastics**

**9**

Natural and Synthetic polymers, plastics – thermosetting and thermoplastic and their general methods of preparation; synthesis of important plastics and their applications-polythene,polypropylene,nylon,polyester,PVC and Bakelite, melanin plastics

**Unit-III: Soaps and Detergents**

**9**

Soap – hard& Soft –manufacture; toilet,laundry,shaving and other types of soaps; cleaning action of soap  
Detergents-their different types and manufacture

**Unit –IV: Fertilizers**

**9**

Fertilizers’ –different types and their requirements; manufacture of urea ammonium phosphate, superphosphate and potassium sulphate and their utilization complexes fertilizers; micronutrients

**Unit –V: Cement**

**9**

Portland and other types of cement; manufacture of Portland cement- wet and dry processes; setting of cement; cement industry in india.

**L: 45 + T: 15, TOTAL: 60 PERIODS**

**References**

1. B.K Sharma, Industrial chemistry, Goel publications,1st revised Edn ,1993
2. M.G, Arora,M,Singh,Industrial chemistry Vol, . 1& 2 Anmol publications. 1st Edn, 1994
3. B.N.Chakrabarthy,industrial chemistry, Oxford & IBH,5th reprint 1991.

**Unit I – Environment and Ecology**

Introduction to environment – concept and scope, environmental segments. Ecosystem and environment. The natural cycles ( $\text{H}_2\text{O}$ ,  $\text{O}_2$ ,  $\text{N}_2$ ) of environment. Environmental pollution and its classification.

**Unit II – Air Pollution**

Atmosphere – composition, structure and evolution; green house effect and global warming; photochemical smog and acid rain. Ozone hole and El Nino phenomenon. Different types of air pollutants and sources; air quality standards.

**Unit III – Water Pollution**

Different types of water pollutants and sources. Eutrophication; heavy metal ions (Hg, Pb and Cr) poisoning; fluoride and defluoridation. Water quality standards.

**Unit IV – Soil Pollution**

Composition of soil; micro and macronutrients; wastes and pollutions in soil; disposal of municipal, medical and industrial wastes. Plants as indicators of soil pollution.

**Unit V- Environmental Restoration**

Environmental restoration; recycling and further use of waste. Conservation of forests and wild life. The state of global environment and earth summit.

**References:**

1. K. De, Environmental Chemistry, New Age publishers, New Delhi, 3, 4 & 5<sup>th</sup> Edn., 2003.
2. K. Sharma and H. Kaur, Environmental Chemistry, Goel Publishing House, Meerut, 3<sup>rd</sup> Edn., 1996.
3. G. S. Sodhi, Environmental Chemistry, Narosa Publishing House, New Delhi, 2000.

**Unit I:****9****Photochemistry:**

Photophysical processes - Jablonski diagram - Photochemical intramolecular reactions of the olefinic bond, geometrical isomerism, cyclization reactions, rearrangement of 1,3- and 1,5-dienes.

Intramolecular reactions of carbonyl compounds: Structural, cyclic and acyclic, Norrish type I and II,  $\alpha$ ,  $\beta$ -unsaturated and  $\beta$ ,  $\gamma$ -unsaturated compounds – cyclohexadienones.

Intermolecular reactions of carbonyl compounds-cycloaddition reaction, dimerizations, Paterno-Buchi reaction.

Photosensitization, photo-oxidation, auto-oxidation, photo-reduction, Barton reaction, photo-Fries rearrangement, di- $\pi$ -methane rearrangement. Photo chemistry of vision.

Pericyclic reactions - conservation of molecular orbital symmetry - electrocyclic and cycloaddition reactions - Sigmatropic rearrangements - applications of correlation diagram - Applications of Frontier Molecular Orbital (FMO) theory. Perturbation Molecular Orbital (PMO) theory and Huckel-Mobius approach to the above reactions - Hofmann-Löffler-Freytag reactions, Ene synthesis, cheletropic reactions.

## **Unit II:**

**9**

### **Molecular Rearrangements**

- a. General mechanistic consideration: Nature of migration, migratory aptitudes, memory effects.
- b. Rearrangement to electron-deficient carbon: Wagner-Meerwein, pinacol-pinacolone, benzil-benzilic acid, Wolff (Arndt-Eistert Synthesis) Demjanov, dienone-phenol.
- c. Rearrangement to electron-deficient nitrogen: Hofmann, Curtius, Schmidt, Lossen Beckmann, Neber
- d. Rearrangement to electron-deficient oxygen: Baeyer-Villiger, Dakin reaction.
- e. Rearrangement proceeding through electron-rich carbon: Stevens, Sommelet-Hauser, Wittig, Favorskii,
- f. Aromatic rearrangements: N-haloanilides, hydroxylamine-aminophenol, von Richter.
- g. Miscellaneous: Bamford-Stevens, Shapiro, Pummerer.

## **Unit III:**

**9**

### **Antibiotics, Vitamins and Steroids**

Antibiotics: Penicillin, chloramphenicol, cephalosporin.

Vitamins: A<sub>1</sub>, A<sub>2</sub>, B<sub>1</sub>, B<sub>2</sub>, H.

Steroids: Androsterone, testosterone, estrone, progesterone.

## **Unit IV:**

**9**

### **Green Chemistry**

Definition – necessity for green chemistry – green chemistry and sustainable environment – principles of green chemistry – atom economy – atom economy vs yield in assessing greenness of organic reactions – example for green chemistry in organic synthesis – methods of greening organic reactions: solvent free reactions, green solvent reactions, green catalysis, microwave assisted reactions – application of ultrasound in organic synthesis - reactions in supercritical fluids – reactions in ionic solvents.

## **Unit V: Advanced Organic Synthesis:**

**9**

Asymmetric synthesis-Definition of enantiomeric and diastereotopic excess-analytical methods to determine ee and de – classification of methods of asymmetric synthesis chiral auxiliaries chiral reagents chiral catalysis.

A systematic analysis of the total synthesis of longifolene, isonootkatone, alphaonocerin, desplarlene and Z-jasmone.

**TOTAL: 60 PERIODS**

## REFERENCES

1. Vertos Chemis, The Conservation of Orbital Symmetry, Gmbh and Asadan Press, 1971.
2. J.M. Coxon and B.Halton, Organic Photochemistry, Cambridge University Press, 1974.
3. Jagdamba Singh and Jaya Singh, Photochemistry and Pericyclic Reaction, New Age International (P) Ltd., New Delhi, 2003.
4. R. Sanghi and M.M. Srivastava – Green Chemistry (Environment Friendly Alternatives), Alpha Science Internaional Ltd, Pangbourne England, 2003.
5. V.K. Ahluwalia – Green Chemistry (Environmentally Beingn Reactions), Ane Books India, New Delhi, 2006.
6. Rashmi Sanshi, M.M. Srivastra – Green Chemistry – Alpha Sciences, 2003.

## CH17A4 INORGANIC MATERIALS AND BIOINORGANIC CHEMISTRY 4 0 0 4

### UNIT-I

9

#### Ceramics

Ceramics – classification, optical waveguides (optical fiber), sol-gel formation for low temperature ceramic formation. Non-oxide ceramics – general aspects, silicon carbide, silicon nitride and boron nitride ceramics. Fabrication of ceramic materials and its challenges. Textile glass fiber (E-glass fiber) and optical fiber manufacture, fabrication and applications.

### Unit II

9

#### Metal oxide pigments

Inorganic pigments: white pigments: TiO<sub>2</sub> pigment, its manufacture, post-treatment and applications; ZnO white, lithopone and ZnS pigments. Coloured pigments: iron oxide pigments – manufacture, oxidation processes and applications; Cr<sub>2</sub>O<sub>3</sub>, chromate, molybdate and ferrocyanide pigments; lustrous, luminescent, magnetic and corrosion protection pigments.

### Unit III

9

#### Inorganic Polymers

General characteristics, degree of polymerization, catenation and heterocatenation, S-N chain one dimensional conductor, isopoly and heteropoly acids (polyoxometallates) and their characteristics and applications (introductory level), phosphazene polymers, homocyclic and heterocyclic inorganic ring systems; Metal clusters: dinuclear, trinuclear, tetranuclear and hexanuclear clusters and their synthesis and properties, polyatomic Zintl anions and cations, infinite metal chains.

## Unit IV –Bioinorganic Chemistry I

9

Non-metals and metals in biological systems, essential and trace elements; classification of metallo-biomolecules, coordination environment and entatic state.

Porphyrin – metal complex systems – chlorophyll and photosynthesis; cytochromes, hemoglobin, myoglobin and dioxygen binding, vitamin B<sub>12</sub> and co-enzyme - *in vivo* and *in vitro* nitrogen fixation.

Iron storage and transport : ferritin, transferrins and siderophores - iron proteins : hemerythrin, cytochrome P450 enzyme, ferredoxin and rubredoxin.

## Unit V – Bioinorganic Chemistry II

9

Copper proteins and Enzymes : plastocyanin, azurin, hemocyanin and ascorbic oxidase - different types of Cu present in proteins and enzymes.

Zinc enzymes : carboxypeptidase A, carbonic anhydrase and superoxide dismutase.

Inhibition and poisoning of enzymes illustrated by xanthine oxidase and aldehyde oxidase.

Toxicity of metals and the role of metallothionins - excess and deficient levels of Cu, and Fe and the consequent diseases - chelate therapy – metal complexes as drugs, anticancer and antiarthritic agents.

Metal complexes as probes of nucleic acids.

**TOTAL: 60 PERIODS**

## REFERENCES

1. H.R. Allcock, Introduction to Materials Chemistry, Wiley, 2008.
2. S.K. Agarwala, Keemti Lal, Advanced Inorganic Chemistry, Pragati Prakashan, 10<sup>th</sup> edn., 2011.
3. A.R. West, Solid State Chemistry and its applications, Wiley, 2004.
4. M.G. Arora, M. Singh, Industrial Chemistry, Anmol Publications, Reprint 2004.
5. Harish Kumar, Industrial Chemistry, Sarup & Sons Reprint 2002.
6. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry, Pearson Education Asia, Reprint 2001.
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**UNIT I****9**

Catalysis phenomenon – mode of action of catalysts – classification of catalysts – Comparison of Homogeneous and Heterogeneous Catalysis. Homogeneous catalysis – general mechanisms; acid-base catalysis – catalytic activity, mechanisms and salt effects.

Enzyme catalysis – influence of substrate concentration, pH, temperature, transient phase kinetics and enzyme mechanisms. Kinetics of inhibition – chain reaction, enzyme catalyzed reactions.

**UNIT II****9**

Catalysis in molecular-scale cavities – structure of crystalline solids – zeolites – families of zeolites; adsorption and diffusion in zeolites – catalysis by zeolites containing metal complexes and clusters; non-zeolite molecular sieves – clays and other layered materials.

Catalysis – catalysts for PTC – mechanism and benefits of PTC – PTC reactions – selected industrial processes with PTC.

**Unit III****9**

Micellar catalysis: effects of micelles on chemical reactions, characteristics of enzymatic reactions, micelle-catalyzed reactions, inhibition in micellar solutions; reverse micelles and microemulsions – catalysis in thermal and photochemical reactions.

**Unit IV****9**

Electrocatalysis – introduction to electrocatalysis and fuel cells – industrial application of catalysis – petroleum refining – distillation, cracking, reforming, hydrotreating, Alkylation and isomerization, steam cracking, ethylene-based processes – ethylene oxide and ethylene glycol, polyethylene, vinyl chloride and PVC; Propylene-based processes – acrylic acid and acrylonitrile, Ziegler-Natta chemistry; C<sub>5</sub>-based processes – butadiene, isobutylene.

**UNIT V****9**

Surface catalysis – introduction – mechanism of surface reactions: Langmuir-Hinshelwood & -Rideal mechanisms; surface structures – single crystal surface of metals, high-surface area amorphous solids; adsorption; functionalized surfaces; catalysis on functionalized surfaces: connection to molecular catalysis; catalysis on metal surfaces, metal oxide surfaces, supported metals, mixed metal oxides, metal sulfides (minimum of one example for each).

**TOTAL: 60 PERIODS****REFERENCES:**

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7. J. M. Smith, Chemical Engineering Kinetics, McGraw Hill, 1971.
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