S.V. NATIONAL INSTITUTE OF TECHNOLOGY SURAT-395007.

Revised Syllabus for B. Tech. II[nd] to B. Tech. IV[th] year

(As approved by 48[th] Senate Meeting held on 26[th] June, 2020)

Sr. No.	B. Tech. (Branch)	Page Number
1.	Chemical Engineering Department	1 to 127
2.	Civil Engineering Department	128 to 312
3.	Computer Engineering Department	313 to 480
4.	Electrical Engineering Department	481 to 622
5.	Electronics Engineering Department	623 to 752
6.	Mechanical Engineering Department	753 to 895

Revised Syllabus for M.Sc. II[nd] to M.Sc. V[th] year

(As approved by 48[th] Senate Meeting held on 26[th] June, 2020)

Sr. No.	M. Sc. (Branch)	Page Number
1.	Applied Chemistry Department	896 to 994
2.	Applied Mathematics & Humanities Department	995 to 1085
3.	Applied Physics Department	1086 to 1187

21/7/2020

Dr. Jyotirmay Banerjee
Dean (Academic)

21/7/2020

Dr. S. R. Gandhi
Director

Revised Syllabus of Five Years Integrated M.Sc. Chemistry (M. Sc. II to V) (Sem. – III to X)

APPLIED CHEMISTRY DEPARTMENT

SARDAR VALLABHBHAI NATIONAL INSTITUTE OF TECHNOLOGY, SURAT

SECOND YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)

M. Sc. - II, SEMESTER – III

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	English & Professional Communication-II	HU-201	3-0-0	03	100	00	00	00	100
2.	Chemistry of Elements	CY-201	3-1-2	05	100	25	30	20	175
3.	Hydrocarbons & Their Functional Groups	CY -203	3-1-2	05	100	25	30	20	175
4.	States and Properties of Matter	CY -205	3-1-2	05	100	25	30	20	175
5.	Economics and Business Management/ Probability and Statistics-I	HU-203/ MA-209	3-1-0	04	100	25	00	00	125
6.	Computational Chemistry Lab.-I	CY -207	0-0-4	02	00	00	60	40	100
Total contact hours per week=29			**Total Credits=24**				**Total Marks=850**		

SECOND YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)

M. Sc. - II, SEMESTER – IV

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Introduction to Life Science	CY-202	3-0-0	03	100	00	00	00	100
2.	Coordination and Bioinorganic Chemistry	CY-204	3-1-2	05	100	25	30	20	175
3.	Stereochemistry and Reaction Mechanism	CY-206	3-1-2	05	100	25	30	20	175
4.	Equilibrium and Changes	CY-208	3-1-2	05	100	25	30	20	175
5.	Modern Physics	PH-212	3-0-0	03	100	00	00	00	100
6.	Computational Chemistry Lab.-II	CY-212	0-0-4	02	00	00	60	40	100
Total contact hours per week=28			**Total Credits=23**				**Total Marks=825**		

ENGLISH & PROFESSIONAL COMMUNICATION-II

L	T	P	C
3	0	0	3

Scheme

HU201

1. Course Outcomes (COs):

At the end of the course the students will able to:

CO1	Express themselves using appropriate vocabulary and grammar.
CO2	Draft scientific reports and formal proposals.
CO3	Comprehend scientific and general content more skilfully and meaningfully.
CO4	Predict human transactions and behavioural modes.
CO5	Communicate effectively through various means and at varied levels.

2. Syllabus:

- **FUNCTIONAL ENGLISH GRAMMAR** **(08 Hours)**
  Language functions, Modals, Tenses, Active and Passive Voice, Conditional Sentences, Concord errors.

- **TECHNICAL WRITING** **(06 Hours)**
  Formal and informal report- Information and recommendation reports, Progress and Periodic Report, Feasibility and trip report. Proposal Writing- Types, logistics of proposals, the deliverables of proposals persuasion and proposal, the structure of the proposal.

- **LISTENING AND READING COMPREHENSION** **(10 Hours)**
  Listening and Note Taking, Paraphrasing, Reading using SQ3R, Predicting, Understanding Gist Reading and Listening General and Scientific Texts and Developing Vocabulary.

- **LANGUAGE THROUGH LITERATURE** **(08 Hours)**
  Short Stories:
  1. The Remarkable Rocket by Oscar Wild.
  2. An Astrologer's Day by R. K. Narayan.
  3. The Case of the Lower Case Letter by Jack Delany.

- **GROUP COMMUNICATION & ACADEMIC WRITING** **(10 Hours)**
  Transactional Analysis; SOP; LOR; Research Paper, Dissertation, Thesis; Types of Group Communication- Seminar, Conferences, Convention, Symposium, Panel Discussion etc.

(Total Lecture Hours: 42)

3. Books Recommended:

1. M. Markel, *Practical Strategies for Technical Communication,* 2nd Edition, Bedford/ St. Martin's, 2016.
2. R. V. Lesikar, M. E. Flatley, *Basic Business Communication Skills for Empowering the Internet Generation,* Tata McGraw Hill publishing company limited. New Delhi 2005.
3. L J. Gurak, J. M. Lannon, *Strategies for Technical Communication in The Workplace* Pearson, 2013.

4. C. L. Bovee, J. V. Thill, M. Chaturvedi, *Business Communication Today*, 9th Edition. Pearson, 2009.
5. W. S. Pfeiffer, T.V.S. Padmaja, *Technical Communication: A Practical Approach*, 6th Edition, Pearson 2013.

CHEMISTRY OF ELEMENTS

CY201

L	T	P	C
3	1	2	5

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Gain knowledge of basic chemistry of main group elements.
CO2	Identify different group elements based on the structure and properties.
CO3	Differentiate between lanthanides and actinides.
CO4	Describe basic concepts of acids and bases.
CO5	Acquire knowledge on properties and use of non-aqueous solvents.

2. Syllabus:

- ***s*- and *p*-BLOCK ELEMENTS** **(12 Hours)**
  s- and *p*- group elements and their compounds: allotropy, structure and bonding, Chemistry and compounds of boron, nitrogen and phosphorous, allotropic forms of carbon, carbides of calcium and silicon, silanes, structure of silicate minerals and silicones. Basic properties of halogens and inter halogen compounds.

- ***d*-BLOCK ELEMENTS** **(08 Hours)**
  Transition elements, position in periodic table, electronic configuration, General characteristics such as oxidation state, size, melting and boiling points, reactivity, ionization energies, magnetic behavior, colour, tendency to form complexes, comparison of properties of first transition series with second and third transition series.

- **LANTHANIDES AND ACTINIDES** **(08 Hours)**
  Electronic configuration and general properties of lanthanides and actinides, extraction and separation of lanthanides and actinides, lanthanide contraction, comparison of *d*- and *f*- block elements, oxidation state, colour and magnetism, trans-uranium elements and their stabilities, coordination chemistry and applications of lanthanide and actinide compounds.

- **ACIDS AND BASES** **(06 Hours)**
  Arrhenius, Bronsted and Lowry concepts of acids and bases. Classification of acids and bases as hard and soft. Pearson's HSAB concept, application of HSAB principle. General trends in acid strength.

- **NON-AQUEOUS SOLVENTS** **(08 Hours)**
  Introduction, solvent classification, effect of the physical properties of the solvent in chemical reactions, acid base reaction, oxidation-reduction reactions, solvolytic reactions, the dielectric constant, the activity coefficient, solubility, ion solvent interactions. Elementary study of ammonia, HF and SO_2 as non- aqueous solvents.

(Total Lecture Hours: 42)

3. Practicals:

- **Inorganic qualitative analysis of inorganic salt mixture containing two cations and two anions**

  Cations: K^+, NH_4^+, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}, Pb^{2+}, Bi^{3+}, Cu^{2+}, Fe^{2+}or Fe^{3+}, Al^{3+}, Co^{2+}, Ni^{2+}, Zn^{2+} and Mn^{2+}.

  Anions: CO_3^{2-}, SO_4^{2-}, S^{2-}, NO_2^-, NO_3^-, Cl^-, Br^-, I^-, CH_3COO^- and PO_4^{3-}.

4. Books Recommended:

1. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Wiley-Blackwell, New Jersey, 1999.
2. T. Moeller, *Inorganic Chemistry: A Modern Introduction*, 2nd Edition, John Wiley & Sons Inc., New York, 1982.
3. F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edition, John Wiley & Sons, New York, 1999.
4. H. Sisler, *Chemistry in Non-Aqueous Solvents*, 3rd Edition, Chapman & Hall, London, 1964.
5. N. N. Greenwood, A. Earnshaw, *Chemistry of the Elements*, 2nd Edition, Butterworth-Heinemann, Massachusetts, 1997.

5. Additional Reading Material:

1. T. Moeller, *The Chemistry of the Lanthanides*, 1st Edition, Chapman & Hall Ltd., London, 1973.
2. C. J. Jones, *d - and f - block Chemistry*, 1st Edition, Royal Society of Chemistry (RSC), Cambridge, 2006.
3. G. L. Miessler, D. A. Tarr, *Inorganic Chemistry*, 3rd Edition, Pearson, 2008.

HYDROCARBONS & THEIR FUNCTIONAL GROUPS

L	T	P	C
3	1	2	5

Scheme

CY203

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Develop knowledge in fundamental aspects of organic chemistry.
CO2	Acquire knowledge on chemical properties of hetero functional groups.
CO3	Acquaint basic knowledge in the chemical properties of carbohydrates and heterocyclic compounds.
CO4	Extend basic knowledge in stability and chemical properties of cycloalkanes.
CO5	Construct practical skills for the purification of solid and liquid organic compounds.

2. Syllabus:

- **HETERO FUNCTIONAL GROUP – I** **(12 Hours)**
  Aliphatic and aromatic halides, hydroxy derivatives, aliphatic alcohols and phenols. Ethers – aliphatic, and aromatic carbonyl compounds. Acid and base-catalyzed ring opening of epoxides, orientation of epoxide ring opening, reactions of Grignard and organolithium reagents with epoxides. Preparation and synthetic applications of ethyl acetoacetate and diethyl malonate, tautomerism.

- **HETERO FUNCTIONAL GROUP – II** **(08 Hours)**
  Aliphatic and aromatic carboxylic acids and their functional derivatives. Nitrogen containing compounds - preparations and reaction mechanisms.

- **CYCLOALKANES** **(06 Hours)**
  Nomenclature, methods of formation, chemical reactions, Baeyer's strain theory and its limitations, theory of strainless ring. Reactions and stereochemistry of substituted cyclohexane.

- **HETEROCYCLIC COMPOUNDS** **(08 Hours)**
  Nomenclature, aromaticity, synthesis, properties, reactivity, uses and canonical structures of: pyrrole, furan, thiophene, pyridine, quinoline and isoquinoline.

- **CARBOHYDRATES** **(08 Hours)**
  Introduction, basic structural features and types of carbohydrates, reactions and conversions, role in biological systems. Introduction to disaccharides, glycosidic bond, structure determination of sucrose, lactose, maltose and gentiobiose.

(Total Lecture Hours: 42)

3. Practicals:

1. Purification of liquid organic compounds
   a. Distillation
   b. Fractional distillation
   c. Steam distillation/Vacuum distillation
   d. Determination of boiling point using distillation
   d. Distillation at reduced pressure

2. Purification of solid organic compounds
   a. Crystallization
   b. Sublimation
   c. Fractional recrystallization

4. Books Recommended:

1. M. A. Fox, J. K. Whitesell, *Organic Chemistry*, 3rd Edition, Jones & Bartlett Learning, Massachusetts, 2004.
2. P. Y. Bruice, *Organic Chemistry*, 3rd Edition, International Edition, Prentice-Hall, New Jersey, 2009.
3. R. T. Morrison, R. N. Boyd, *Organic Chemistry*, 7th Edition, Prentice Hall, New Jersey, 2011.
4. A. Streitwieser, Jr., C. H. Heathcock, *Introduction to Organic Chemistry*, 4th Edition, MacMillan, New York, 1998.
5. R. R. Gupta, M. Kumar, V. Gupta, *Heterocyclic Chemistry*, Volume 2, 1st Edition, Springer India Pvt. Ltd., New Delhi, 2009.

5. Additional Reading Material:

1. T. W. G. Solomons, C. B. Fryhle, *Organic Chemistry*, 9th Edition, Wiley India Pvt. Ltd., Navi Mumbai, 2009.
2. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, Pearson India, Noida, 5th Edition, 2005.
3. P. Sykes, *A Guidebook to Mechanism in Organic Chemistry*, Pearson (publisher), 6th Edition, 2003.

STATES AND PROPERTIES OF MATTER

L	T	P	C
3	1	2	5

Scheme

CY205

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Recognize the basic theoretical knowledge of solids and liquids applicable in multidisciplinary fields.
CO2	Recall basics of solutions and apply thermodynamic treatment in solutions.
CO3	Accumulate a fundamental knowledge of colloidal state.
CO4	Classify state of matter based on physical properties.
CO5	Perform the experiments related to physical chemistry approach which includes solution preparation, and titration dealing with conductometry, colorimetry, and pH-metry.

2. Syllabus:

- **SOLID STATE** **(10 Hours)**

  Unit cell, Bravais lattice and its types, Miller indices, X-ray diffraction, Bragg's law and its derivation, Calculation of basis per unit crystal, volume, density per unit cell, Diffraction techniques (Qualitative treatment only): single crystal and powder, Structure elucidation of ZnS (Wurtzite and blende), Specific heat of solids (Dulong Petit law, Einstein's theory, Debye correction qualitatively), Band theory, Superconductivity, Point defects (Schottky and Frenkel).

- **LIQUID STATE** **(10 Hours)**

  General features of liquid state (short and long range order/disorder, hole theory), Vapor pressure, Young and Laplace equation, Surface tension, Surface energy, Excess pressure, Capillarity phenomenon, Work of adhesion and cohesion, Contact angle, Spreading of liquids, Temperature dependence of surface tension, measurement of surface tension, Viscosity of liquids, Temperature dependence of viscosity of liquids, Poiseuille's equation and Measurement of surface viscosity, Numericals.

- **COLLOIDAL CHEMISTRY - I** **(10 Hours)**

  Colloids: Definition, general properties of colloids (optical and electrical), Types of colloidal system, Classifications of colloids, Colloidal state, multimolecular, macromolecular and associated colloids, Stability and kinetics of colloids, Zeta potential. Rayleigh equation and its outcomes, Sol, Lyophobic and lyophilic sol, Size range and its preparation.

- **SOLUTION** **(12 Hours)**

  Types of solutions, Ideal and non-ideal solutions, The thermodynamic properties of ideal solutions, Molecular interpretation of the entropy of mixing, Vapor pressure and thermodynamics of non-ideal systems, general considerations (mixing and excess functions), Solvents of non-ideal solutions, the activity and activity coefficients, solutes of non-ideal solutions, The Gibbs-Duhem equation and determination of solute activity, Partial and apparent molar properties (chemical potential, enthalpy and volume), Methods for their determinations.

(Total Lecture Hours: 42)

3. Practicals:

1. Preparation of the solution, calibration, Standard Deviation.
2. Determination of the partition coefficient of Benzoic acid in Kerosene.
3. To find out the strength of HCl solution (N/10) by conductometric titration against standard NaOH solution.
4. To verify Beer's law for $K_2Cr_2O_7$ solution spectrophotometrically and determine the unknown concentration.
5. To determine the dissociation constant of weak monobasic acid by pH-metric titration.
6. Determination of surface tension of a given solution by drop weight (stalagnometer) method.
7. Complexometric determination of total hardness of water by EDTA titration.
8. To determine rate constant of decomposition of H_2O_2 by acidified KI solution.

4. Books Recommended:

1. B. R. Puri, L. R. Sharma, M.S. Pathania, *Principles of Physical Chemistry*, 47th Edition, Vishal Publications, New Delhi, 2017.
2. G. Raj, *Advanced Physical Chemistry*, 4th Edition, Goel Publishing House, Meerut, 1990.
3. A. R. West, *Solid State Chemistry and its Applications*, 2nd Edition, student edition, John Wiley & Sons, New York, 2014.
4. P. Atkins, J. de Paula, J. Keeler *Atkins' Physical Chemistry*, 11th Edition, 2018.
5. K. J. Laidler, *Chemical Kinetics*, 3rd Edition, Person, 2003.

ECONOMICS AND BUSINESS MANAGEMENT

L	T	P	C
3	1	0	4

HU203

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Develop managerial skills.
CO2	Acquire skills related to various functional areas of management (marketing management, financial management, operations management, personnel management etc.)
CO3	Build knowledge about modern management concepts (ERP, SCM, e-CRM, etc.)
CO4	Record experiential learning in management through real life examples and case study etc.
CO5	Apply knowledge of economics and business management aspects in their field.

2. Syllabus:

- **ECONOMICS** **(08 Hours)**
  Introduction to Economics, Micro & Macro Economics, Applications & Scopes of Economics, Demand Analysis, Demand Forecasting, Factors of Production, Types of Cost, Market Structures, Break Even Analysis

- **MANAGEMENT** **(12 Hours)**
  Introduction to Management, Features of Management, Nature of Management, Development of Management Thoughts – Scientific Management By Taylor & Contribution of Henry Fayol, Coordination & Functions of Management, Centralization & Decentralization, Decision Making; Fundamentals of Planning; Objectives & MBO; Types of Business Organizations: Private Sector, Public Sector & Joint Sector; Organizational Behavior: Theories of Motivation, Individual & Group Behavior, Perception, Value, Attitude, Leadership

- **FUNCTIONAL MANAGEMENT** **(18 Hours)**
  Marketing Management: Core Concepts of Marketing, Marketing Mix (4p), Segmentation – Targeting – Positioning, Marketing Research, Marketing Information System, Concept of International Marketing, Difference Between Domestic Marketing & International Marketing; Operations Management: Introduction to Operations Management, Types of Operation Systems, Types of Layouts, Material Handling, Purchasing & Store System, Inventory Management; Personnel Management: Roles & Functions of Personnel Manager, Recruitment, Selection, Training, Industrial Dispute, Collective Bargaining; Financial Management: Goal of Financial Management, Key Activities In Financial Management, Organization of Financial Management, Financial Institutions, Financial Instruments, Sources of Finance

- **MODERN MANAGEMENT ASPECTS** **(04 Hours)**
  Introduction to ERP, e – CRM, SCM, RE – Engineering, WTO, IPR Etc.

(Total Lecture Hours: 42)

3. Books Recommended:

1. L. M. Prasad, *Principles & Practice of Management*, 8th Edition, Sultan Chand & Sons, 2015.
2. T. R. Banga, S. C. Shrama, *Industrial Organisation & Engineering Economics*, 25th Edition, Khanna Publishers, 2015.
3. E. E. Adam, R. J. Ebert, *Production and Operations Management*, 5th Edition, Prentice Hall of India, 2012.
4. P. Kotler, K. L. Keller, A. Koshi, M. Jha, *Marketing Management – A South Asian Perspective*, 14th Edition, Pearson, 2014.
5. P. C. Tripathi, *Personnel Management & Industrial Relations*, 21st Edition, Sultan Chand & Sons, 2013.

4. Additional Reading Material:

1. P. Chandra, *Financial Management*, 9th Edition, Tata McGraw Hill, 2015.

PROBABILITY AND STATISTICS-I

MA209

L	T	P	C
3	1	0	4

Scheme

1. Course Outcomes (Cos):

At the end of the course students will be able to:

CO1	Recognize the basic ideas of measures of central tendency, dispersion and their applications.
CO2	Acquire the knowledge of various Probability distributions and their applications.
CO3	Compute correlation, regression and confidence intervals to formulate hypotheses.
CO4	Apply statistical techniques for sampling of big data.
CO5	Demonstrate the statistical techniques for estimation of data.

2. Syllabus:

- **PROBABILITY AND DESCRIPTIVE MEASURES** **(07 Hours)**
  Historical development, Basic Concepts, rule, Measures of Central Tendency, Measures of Dispersion, Tchebycheff's theorem and Empirical Rule Measures of relative standing, some principles of statistical model. Random variables, Probability, conditional probability and Baye's theorem. Expected value, moment generation function and variance of a random variable, covariance.

- **PROBABILITY DISTRIBUTIONS** **(08 Hours)**
  Probability Distributions: binomial and multinomial distribution, geometric distribution, hypergeometric distribution, normal distribution, gamma distribution, exponential distribution, negative binomial distribution, Two dimensional distribution, joint and marginal distribution.

- **CENTRAL LIMIT THEOREM** **(04 Hours)**
  Central limit theorem for Bernoulli trails, normal approximation to binomial, the general central limit theorem.

- **CORRELATION, REGRESSION AND TESTING OF HYPOTHESIS** **(08 Hours)**
  Correlation, multiple correlation, Linear Regression, Properties of the Least Square Estimators, Inferences concerning the Regression coefficients, Analysis of variance for Linear Regression, Testing the usefulness of the Linear Regression Model. Multiple regression, Testing the significance of the regression coefficients, Testing of linear hypothesis, Bias in the regression estimators due to choice of wrong model.

- **SAMPLING METHODS** **(07 Hours)**
  Random Sampling and Methods of Sampling, Sampling Distribution and Standard Error, Sampling Distribution of the Sample Mean, Central Limit Theorem, Sampling Distribution of the Sample Proportion, Sampling Distribution of the difference between two sample means and Sampling Distribution of the difference between two sample proportions.

- **ESTIMATION METHODS** **(08 Hours)**
  Point Estimation, Interval Estimation, Confidence Interval, Large Sample Confidence Interval for a Population Mean μ, Large Sample Confidence Interval for a Population Proportion, estimating the

difference between two Population means, estimating the Difference between two Binomial proportions, Maximum Likelihood Estimation.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. W. Mendenhall, R. J. Beaver, B. M. Beaver, *Introduction to Probability & Statistics*, 12th Edition, India Edition, Thomson, 2012.
2. G. Smith, *Essential Statistics, Regression & Econometrics*, 2nd Edition, 2015.
3. C. Grinstead, J. Snell, *Introduction to Probability*, American Mathematical Society, 2006.
4. Montgomery, *Applied Statistics and Probability for Engineers*, 6th Edition, Wiley India Pvt Ltd, 2014.
5. R. E. Walpole, S. L. Myers, K. Ye, *Probability& Statistics for Engineers & Scientists*, 9th Edition, Pearson, 2012.

COMPUTATIONAL CHEMISTRY LAB. – I

CY207

L	T	P	C
0	0	4	2

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Develop computational chemistry literacy.
CO2	Explore the importance of computational chemistry software.
CO3	Hands-on experience with some standard computational software.
CO4	Compute 3D structure of molecules.
CO5	Calculate electronic and thermodynamic properties.

2. Syllabus:

- **INTRODUCTION** **(12 Hours)**
  Practice with some commonly used drawing and visualization softwares: Chemdraw, Chemsketch, Avogardo, molden etc; Scope of computational chemistry; Demonstration of basic theory for molecular mechanics and quantum mechanical calculations; Introduction to some quantum mechanical softwares: Gaussian; Hyperchem; Spartan; Gamess; Molecular dynamic softwares: Gromacs, Lammps, Amber, MDynaMix; Molecular docking softwares: Autodock.

- **WORKING WITH COMPUTATIONAL SOFTWARE (OPTIMIZATION)** **(22 Hours)**
  Hands-on experience with Gaussian and GaussView; Single point energy calculations, geometry optimization with MM, Semi-empirical, Ab-Initio and DFT methods, Effects of basis sets, location of transition states, Frequency calculations, conformational analysis, predicting molecular stability, studying chemical reactions and reactivity, modeling in solutions.

- **CALCULATING ELECTRONIC AND THERMODYNAMIC PROPERTIES** **(22 Hours)**
  Predicting thermochemistry: Thermal energy: E (Thermal), Constant volume molar heat capacity (Cv), Entropy (S), Free Energy (sum of electronic and thermal Free Energies), Enthalpy (sum of electronic and thermal Enthalpies), Atomization energies, Electron Affinity, Ionization Potential, Proton Affinity, Electrostatic potential Map and electron density, Mulliken's Atomic charges. NBO's, molecular orbitals and band gap calculations, dipole moment, polarizability, volume.

(Total Contact Hours: 56)

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3. Practicals:

1. To demonstrate the use of chemical structure drawing program ChemDraw and molecular modeling counterpart Chem3D to draw and manipulate different organic chemistry structures.
2. Practice for drawing chemical structure with ChemDraw and Chem3D.
3. To demonstrate the theories and applications of the computational tools in understanding chemical phenomena.
4. Practice with Gaussian 09W ad Gaussview: predicting least strain structure of cyclohexane and substituted cyclohexane.
5. Optimization of the various conformations of propene, vinyl alcohols, vinyl amine by semi-empirical, HF and DFT methods.

6. To calculate the structure of a transition state between the two stable structures of 1,3-butadiene.
7. To calculate various thermodynamic properties of naphthalene.
8. To calculate Mulliken's Atomic charges. NBO's, molecular orbitals and band gap calculations, Electrostatic potential Map and electron density with suitable examples
9. To calculate the atomization energies and Electron Affinity.
10. To calculate the Ionization Potential and Proton Affinity.

4. Books Recommended:

1. J. B. Foresman, A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian, Inc., Pittsburgh, 1996.
2. D. Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*; John Wiley & Sons, inc: USA, 2001.
3. F. Jensen, *Introduction to Computational Chemistry*, 2nd Edition, John Wiley & Sons, inc: England, 2007.
4. A. Tomberg, *Gaussian 09w Tutorial An Introduction to Computational Chemistry Using g09w and Avogadro Software.*
5. C. J. Cramer, *Essentials of Computational Chemistry: Theories and Models,* 2nd Edition, Wiley & Sons, New York, 2002.

SECOND YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)

M. Sc. - II, SEMESTER – IV

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Introduction to Life Science	CY-202	3-0-0	03	100	00	00	00	100
2.	Coordination and Bioinorganic Chemistry	CY-204	3-1-2	05	100	25	30	20	175
3.	Stereochemistry and Reaction Mechanism	CY-206	3-1-2	05	100	25	30	20	175
4.	Equilibrium and Changes	CY-208	3-1-2	05	100	25	30	20	175
5.	Modern Physics	PH-212	3-0-0	03	100	00	00	00	100
6.	Computational Chemistry Lab.-II	CY-212	0-0-4	02	00	00	60	40	100
Total contact hours per week=28			**Total Credits=23**				**Total Marks=825**		

INTRODUCTION TO LIFE SCIENCE

CY202

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Identify basics of life science.
CO2	Distinguish on interfaces between chemistry and biology.
CO3	Acquire knowledge about prokaryotic Diversity.
CO4	Explain cell structure and metabolisms.
CO5	Apply fundamental knowledge on bacteria and microorganisms.

2. Syllabus:

- **INTRODUCTION TO CELL BIOLOGY** **(09 Hours)**
  Origin of life, Discovery of cell and Cell Theory; Comparison between plant and animal cells; Cell wall; Plasma membrane; Cytoskeleton; Protoplasm; Mitochondria; Chloroplast; ER; Golgi complex; Lysosome, Ribosome; Nucleus; Chemical components of a cell; Cell division and cell cycle: Mitosis and meiosis (different phases in cell division), their regulation, steps in cell cycle, and control of cell cycle.

- **HEREDITY AND VARIATION** **(09 Hours)**
  Mendelian inheritance; deviations from Mendelism – incomplete dominance, co-dominance, (example of heredity and variation multiple alleles and inheritance of blood groups), chromosome theory of inheritance; chromosomes and genes. DNA as genetic material; Structure of DNA and RNA; DNA packaging; DNA replication; Central dogma; transcription, genetic translation.

- **PROKARYOTIC DIVERSITY** **(09 Hours)**
  Prokaryotic Diversity: Importance of Taxonomy, Nomenclature and Bergey's Manual; **Archaea:** Archaea as earliest Life forms; Halophiles; Methanogens; Hyperthermophilic archaea; Thermoplasma; **Bacteria:** Purple and green bacteria; Cyanobacteria; Acetic acid bacteria; Spirilla; Spirochaetes; Pseudomonads; Lactic and propionic acid bacteria; Mycobacteria; Rickettsias, Chlamydias and Mycoplasms; **Viruses:** Bacterial, Plant, Animal and Tumor viruses; Discovery, classification and structure of viruses; **Eukarya:** Algae, Fungi, Slime molds and Protozoa.

- **STRUCTURE AND FUNCTION OF BACTERIAL CELL** **(05 Hours)**
  The cell wall of bacteria containing peptidoglycan and related molecules; the outer membrane and cytoplasmic membrane. Water and ion transport across membrane. Membrane structure & transport – Models of membrane structure, Membrane lipids, proteins and carbohydrates; Solute transport by Simple diffusion, Facilitated diffusion and Active transport.

- **METABOLIC DIVERSITY AND SYNTROPY AMONG MICROORGANISMS (10 Hours)**
  Bacterial Growth and Diversity, Bacterial cell cycle, Measurements and Isolation of Microorganism – Different Cultures – Media and Techniques of Staining (Gram-negative and Gram-positive bacteria); Introduction to photosynthesis in microorganisms (Role of Chlorophylls, carotenoids and phycobilins); Calvin cycle; Chemolithotrophy; Oxidation-reduction by bacteria: (Hydrogen - iron -

nitrite ,– oxidizing bacteria; Nitrate and sulfate reduction); Methanogenesis and acetogenesis: Fermentations – diversity and syntropy.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. D. O. Morgan, *The cell cycle: Principle of controls*, 1st Edition, New Science Press, 2007.
2. D. M. Prescott, *Reproduction in Eukaryotic cells*, 1st Edition, Academic press, 1976
3. R. Y. Stainer, J. L. Ingraham, M. L. Wheelis, P. R. Painter, *General Microbiology*, 5th Edition, The MacMillan Press Ltd, 1987.
4. D. L. Nelson, M.M. Cox, *Lehninger's Principles of Biochemistry,* 5th Edition, CBS Publications, 2008.
5. M. J. Pelczar, R. D. Reid, *Microbiology,* 5th Edition, Tata McGraw Hill, 1986.

COORDINATION AND BIOINORGANIC CHEMISTRY

L	T	P	C
3	1	2	5

Scheme

CY204

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Describe the fundamentals of coordination compounds.
CO2	Generalize basic theories on bonding in coordination compounds.
CO3	Identify metal hydrides and their importance.
CO4	Explain role of metal ions in biological processes.
CO5	Explore the use of metal ions and complexes in medicine.

2. Syllabus:

- **COORDINATION CHEMISTRY** **(20 Hours)**

  Ligands, coordination numbers, coordination sphere, Nomenclature, Werner's theory, EAN, Chelates, isomerism in coordination compounds, Valence Bond theory, octahedral, tetrahedral and square planner complexes, Crystal field theory (CFT), Crystal field splitting of d-orbitals in octahedral, square planar and tetrahedral complexes, CFSE, factors affecting the magnitude of Δ, spectrochemical series, Jahn-Teller effect and other crystal-field effects, limitations of CFT, LFT, nephelauxetic series, molecular orbital theory of coordination chemistry, sigma and pi bonding in complexes, Magnetism of complexes.

- **BIOINORGANIC CHEMISTRY** **(12 Hours)**

  Biological roles of alkali and alkaline earth metal ions, ions transport (active) across biological membrane and its significance, mechanism of Na^+/K^+-ions pump; Metalloproteins and enzymes: role of metal ions in the active sites, structure and functions of enzymes containing Zn, Mg, Ca and Cu; Carbonic anhydrase and carboxypeptidase, Zinc finger proteins; Bioinorganic chemistry of copper-electron transfer proteins, dioxygen transport and metabolism, Plastocyanin, haemocyanin, Ascorbate oxidase; nitrogen fixation, Essential and toxic metals ions in different biological processes, Porphyrins, Metalloporphyrins, haemoglobin, and myoglobin, ferritin and transferrin. Structures and functions of cytochromes, cytochrome c; iron-sulfur proteins (ferredoxines) and cytochrome c oxidase, photosynthesis: chlorophyll; Metal complexes in medicine

- **INORGANIC HYDRIDES** **(10 Hours)**

  Classification, preparation, bonding and their applications. Transition metal compounds with bonds to hydrogen, carbonyl hydrides and hydride anions. Classification, nomenclature, Wades Rules, preparation, structure and bonding in boron hydrides (boranes), carboranes, metalloboranes and metallocarboranes.

(Total Lecture Hours: 42)

3. Practicals:

1. **Iodo / Iodimetric Titrations**
   a. Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).
   b. Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically

2. **Complexometric Titrations (EDTA titrations)**: Titration of mixtures using masking and demasking agents.
   a. Complexometric estimation of (i) Mg^{2+} and (ii) Zn^{2+} using EDTA
   b. Estimation of total hardness of water samples
3. **Argentometry**
   a. Estimation of Cl^- (i) By Mohr's method, (ii) By Volhard's method, (iii) By Fajan's method.
   b. Estimation of copper as CuSCN.
   c. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$ through,
   (i) Heterogeneous and (ii) Homogeneous media.
   d. Estimation of Al^{3+} by precipitating with oxime and weighing as $Al(oxine)_3$ (aluminiumoxinate).

4. Books Recommended:

1. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Wiley-Blackwell, New Jersey, 1999.
2. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, *Inorganic Chemistry-Principles of Structure and Reactivity*, 4th Edition, Pearson Education, London, 2006.
3. S. J. Lippard, J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, 1994.
4. W. Kaim, B. Schewederski, A. Klein, *Bioinorganic Chemistry -- Inorganic Elements in the Chemistry of Life: An Introduction and Guide*, 2nd Edition, John Wiley & Sons, New York, 2013.
5. E. Crabb, *Metals and life*, 1st Edition, RSC, 2009.

5. Additional Reading Material:

1. R. Crichton, *Biological Inorganic Chemistry: A new introduction to molecular structure and function*, 2rd Edition, Elsevier, 2012.
2. P. Atkins, Shriver, *Inorganic Chemistry*, 5th Edition, Oxford, 2009.

STEREOCHEMISTRY AND REACTION MECHANISM

L	T	P	C
3	1	2	5

Scheme

CY206

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Demonstrate the stereochemistry of simple organic molecules.
CO2	Explain the stereospecific and stereo selective synthesis.
CO3	Acquire the basic concepts and knowledge of various substitution reactions.
CO4	Gain the knowledge in the reaction mechanisms and how the factors are influenced in substitution reactions.
CO5	Apply practical knowledge in the identification of organic compounds.

2. Syllabus:

- **STEREOCHEMISTRY** **(08 hours)**
  Prochirality, chirality, CIP nomenclature of more than one chiral center, methods of resolution, stereospecific and stereoselective synthesis, asymmetric synthesis, optical activity in absence of chiral carbon (biphenyl, allenes and spiranes), chirality due to helical shape.

- **AROMATIC ELECTROPHILIC SUBSTITUTION** **(09 Hours)**
  Aromaticity, Mobius and Huckel rule for polyenes and annulene, effect of substituents on reactivity, theory of activity and deactivity effects. Arenium ion mechanism, orientation and reactivity, ortho and pararatio, Ipso effect, orientation in other ring systems, calculation of partial rate factor, quantitative treatment of reactivity in substrates and electrophiles. Chemistry of naphthalene, anthracene and phenanthrene.Carcinogenicity.Nonbenzenoid aromatic compounds.

- **NUCLEOPHILIC SUBSTITUTION REACTIONS** **(11 Hours)**
  SN^2, SN^1, mixed SN^1 and SN^2 and SET mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon.Reactivity effects of structure, attacking nucleophile, leaving group and reaction mechanism, solvent effect, phase transfer catalyst, ambident nucleophile and regioselectivity. Energy profile diagram, diazonium coupling Vilsmeier reaction, Gattermann – Koch reaction, and other carbocyclic rings. $ArSN^1$ and benzyne mechanisms, reactivity effect of substrate structure, leaving group and attacking nucleophile.Introduction of azide, phosphorus and sulphur nucleophiles.

- **REACTION MECHANISM** **(07 Hours)**
  Investigation of reaction mechanism, SN^1 mechanism, nucleophilic substitution of allylic halides. Neighbouring group mechanism, neighbouring group participation by π- and σ- bonds, -OH, $-NH_2$, -COO, -halogen and aromatic ring, stereochemistry of reactions.

- **ELIMINATION REACTIONS** **(07 Hours)**
  E_1, E_2 and E_1CB mechanism and their spectrum orientation of the double bond, reactivity effects of substrate structures, attacking base, leaving groups and the medium, mechanism and orientation in pyrolytic elimination. Von-Richter and Sommlet-Houser rearrangement.

(Total Lecture Hours: 42)

3. Practicals:

1. Identification of single organic compounds (I to VII).

4. Books Recommended:

1. E. L. Eliel, S. H. Wilen, *Stereochemistry of Organic Compounds*, 1st Edition, John Wiley & Sons, New York, 2008.
2. D. Nasipuri, *Stereochemistry of Organic Compounds: Principles and Applications*, 2nd Edition, New Age International (P) Limited, New Delhi, 2005.
3. M. B. Smith, J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 6th Edition, Wiley-Interscience, New Jersey, 2012.
4. A. Streitwieser, Jr., C. H. Heathcock, *Introduction to Organic Chemistry*, 4th Edition, MacMillan Publishing Company, New York, 1998.
5. J. Clayden, N. Greeves, S. Warren, *Organic Chemistry*, 2nd Edition, Oxford University Press, Oxford, 2012.

5. Additional Reading Material:

1. K. P. C. Volhardt, N. E. Schore, *Organic Chemistry: Structure and Function*, 7th Edition, W. H Freeman & Co., 2014.
2. H. Maskill (Ed.), *The Investigation of Organic Reactions and their Mechanisms*, 1st Edition, Blackwell Publishing Ltd. Oxford, 2006.
3. R. L. Shriner, C. K. F. Hermann, T. C. Morrill, D. Y. Curtin, R. C. Fuson, *Systematic Identification of Organic Compounds*, 8th Edition, John Wiley & Sons, New York, 2004.
4. P. S. Kalsi, *Stereochemistry Conformation and Mechanism*, 8th Edition, New Age International, 2015.
5. Jerry March, *Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, 7th Edition, Wiley-Blackwell; 4th Revised Edition, 2015.

EQUILIBRIUM AND CHANGES

CY208

L	T	P	C
3	1	2	5

Scheme

1. Course Outcomes (Cos):

At the end of the course students will be able to:

CO1	Demonstrate successive relationships between varied equilibria constants and apply the mechanism of phase rule with phase diagram for various systems.
CO2	Explain the thermochemistry in deep and calculate heat of a reaction.
CO3	Enumerate basics of EMF series and its application.
CO4	Accumulate a deep knowledge in surface phenomena applicable in multidisciplinary areas.
CO5	Perform the experiments related to physical chemistry approach which includes Kinetics, Conductometry, Colorimetry, pH-metry, Potentiometry and Titration .

2. Syllabus:

- **THERMOCHEMISTRY** **(08 Hours)**

  Standard state, standard enthalpy of formation, Hess's law and its applications, heat of reaction at constant pressure and at constant volume, enthalpy of neutralization, bond dissociation energy and its calculation from thermochemical data, Kirchhoff's equation, Joule Thomson effect, inversion temperature. Nernst distribution law: Derivation, application and limitations, distribution coefficient, Henry's law, solvent extraction. Numericals.

- **IONIC EQUILIBRIA** **(08 Hours)**

  Ostwald's dilution law and its derivation, Strength of acids and bases on their dissociation constants, ionic product of water, pH scale, measurement of pH, Common Ion effect, buffer capacity, buffer in biological systems, Henderson's equations, hydrolysis of salts, hydrolysis constant, relationship between K_h, K_a, K_b, K_w, degree of hydrolysis, acid base indicators, concept of solubility product. Numericals.

- **PHASE EQUILIBRIA** **(08 Hours)**

  Definition of Phase, Phase boundaries, Components, degree of freedom, phase rule, Thermodynamic condition for phase equilibrium, Phase rule and its derivation, Phase equilibrium for one component system (for example H_2O, S, CO_2), First and second order phase transition, Clapeyron equation, Clausius-Clapeyron equation, Liquid vapor equilibrium for two component system, Critical solution temperature, Completely immiscible systems, Simple eutectic systems: Zn-Cd, Pb-Ag.

- **ELECTROCHEMISTRY – II** **(09 Hours)**

  Single electrode potential, Hydrogen electrode, Galvanic cell, EMF series, Nernst equation, Reversible electrodes, metal-metal ion electrodes, Calomel electrode, Standard Hydrogen Electrode (SHE), Oxidation-Reduction electrodes, Potentiometric titration, Application of electrochemistry in Corrosion control by cathodic protection, batteries, and fuel cells, Interface of chemical sciences with other disciplines. Numerical.

- **SURFACE CHEMISTRY** **(09 Hours)**

  Adsorption (Physisorption and chemisorption), adsorption isotherms, BET equation for estimation of surface area. Solid-liquid interfaces, Contact angle and wetting, Solid-gas interface, Surface

active agents and their classification, Gibbs adsorption from solution, Critical micellar concentration (CMC), micelles, thermodynamics of micellization, reverse micelles.

(Total Lecture Hours: 42)

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3. Practicals:

1. Determine the rate constant and the order of the reaction of $KBrO_3$ and KI in acid medium.
2. Determination of the partition coefficient of iodine (I_2) between carbon tetrachloride (CCl_4) and water.
3. Determination of ionization constant of a weak acid by Conductometric method.
4. Determination of equivalent conductance (Λ_∞) of weak monobasic (acetic acid) and verify Ostwald's Dilution Law.
5. To find out the strength of HCl solution (N/10) by pH-metric titration against standard NaOH solution.
6. To study the kinetics of saponification of ester by conductometric method.
7. Determination of absorbance of $K_2Cr_2O_7$ and $KMnO_4$ and their mixture using colorimetry. Further verify Beer's law for them. Also determine their unknown concentration in given sample solution.
8. To determine individual concentration of Cu^{2+} and Ca^{2+} in the mixture using EDTA.

4. Books Recommended:

1. G. M. Barrow, *Physical Chemistry*, 6th Edition, McGraw-Hill, New Delhi, 1996.
2. B. R. Puri, L. R. Sharma, M. S. Pathania, *Principles of Physical Chemistry*, 47th Edition, Vishal Publications, New Delhi, 2017.
3. G. Raj, *Advanced Physical Chemistry*, 4th Edition, Goel Publishing House, Meerut, 1990.
4. S. K. Maity, N. K. Ghosh, *Physical Chemistry Practical*, 1st Edition, New Central Book Agency (P) Ltd., Kolkata, 2012.
5. S. Glasstone, *An Introduction to Electrochemistry,* Maurice Press, 2011.

MODERN PHYSICS

L	T	P	C
3	0	0	3

PH212

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Enumerate the limitations of Classical Physics and need for a new theory.
CO2	Identify the relevance of concepts of Modern Physics and their implications.
CO3	Interpret the results of Quantum Physics and relevant laws.
CO4	Explain the Black body radiation laws, duality of waves and matter and their significance.
CO5	Analyze the relevant problems of modern physics including Lasers.

2. Syllabus:

- **LIMITATIONS OF CLASSICAL PHYSICS AND INTRODUCTION TO QUANTUM PHYSICS** **(08 Hours)**
  Classical physics as an approximate of quantum physics, limitations of classical Physics at microscopic levels.

- **BASICS OF QUANTUM PHYSICS AND QUANTUM MECHANICS** **(08 Hours)**
  Black body radiation, Wein's, Rayleigh-Jeans, and Planck's laws, Dual nature, Atomic models, Exclusion principle, and quantum numbers, The wave equation.

- **PHOTOELECTRIC EFFECT AND COMPTON EFFECT** **(06 Hours)**
  Photoelectric effect and Einstein's explanation, Compton effect and equation of Wavelength.

- **X – RAYS** **(08 Hours)**
  Production and characteristics of X-rays, X-ray diffraction and Bragg's law.

- **LASERS, FIBRE OPTICS & APPLICATIONS** **(12 Hours)**
  Laser fundamentals, types of lasers, Basics of Fibre optics, types of fibres, applications.

(Total Lecture Hours: 42 Hours)

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3. Books Recommended:

1. A. Beiser, *Concept of the Modern Physics*, Tata McGraw Hill, 2008.
1. A. Ghatak, *Optics*, Tata McGraw Hill, 2005.
2. M. R. Wehr, J. A. Richards, T. W. Adair, *Physics of the Atom*, Addison – Wesley, 1984.
3. R. Harris, *Modern Physics*, Addison-Wesley/ Pearson,2/E ,2007
4. M. Born, E. Wolf, *Principles of Optics*, Cambridge Uni. Press, 2000.

COMPUTATIONAL CHEMISTRY LAB. – II

L	T	P	C
0	0	4	2

CY212

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Calculate molecular spectroscopy
CO2	Enumerate excited state geometry and properties
CO3	Compare theoretical and experimental spectra
CO4	Express molecular dynamic simulations
CO5	Explain molecular docking with suitable examples

2. Syllabus:

- **CALCULATING SPECTROSCOPIC PROPERTIES** **(20 Hours)**
  IR and Raman spectra, DFT and TD-DFT calculations, UV-Vis and emission spectra, Excited states properties and structure, NMR spectra and spin-spin coupling constants, Vibrational circular dichroism (VCD), Raman optical activity (ROA), Electronic circular dichroism (ECD), Optical rotary dispersion (ORD), Hyperfine spectra (microwave spectroscopy).

- **MOLECULAR DYNAMIC SIMULATIONS** **(18 Hours)**
  Discussion on the
  basic theories and algorithms used for dynamic simulations, Dynamics of drugs, biomolecules, drug-receptor complexes, Molecular dynamics in performing conformational search and other applications. Estimation of free energy from dynamical methods, Hand-on experience with some standard software with suitable examples.

- **MOLECULAR DOCKING** **(18 Hours)**
  Discussion on the basic theories and algorithms used on docking, Rigid docking, flexible docking, manual docking. Hand-on experience with Autodock and other Dock software, Applications.

(Total Contact Hours: 56)

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3. Practical:

1. Introduction to use of computation tools in predicting molecular spectroscopy.
2. To calculate IR using the Gaussian 09W and to demonstrate the other importance of frequency calculations.
3. To calculate Raman and polarizability using the Gaussian 09W
4. To calculate the UV Vis spectrum of acrolein using CIS/TDDFT method.
5. To calculate the emission spectra of phenol using the Gaussian 09W.
6. Theoretical predicting 1H and 13C NMR spectra and spin-spin coupling constants of ethanol.
7. To calculate vibrational circular dichroism (VCD) and Raman optical activity (ROA) using the Gaussian 09W.
8. To calculate Electronic circular dichroism (ECD), Optical rotary dispersion (ORD) using the Gaussian 09W.

9. Demonstration to perform molecular dynamic simulation with Gromacs/Amber.
10. Demonstration to perform molecular docking with Autodock.

3. Books Recommended:

1. J. B. Foresman, A. Frisch, *Exploring Chemistry with Electronic Structure Methods*, 2nd Edition, Gaussian, Inc., Pittsburgh, 1996.
2. D. Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems;* 1st Edition, John Wiley & Sons, inc: USA, 2001.
3. A. R. Leach, *Molecular Modelling: Principles and Applications*, 2nd Edition, Prentice Hall, 2001.
4. E. G. Lewars, *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics,* 3rd Edition, Springer, 2011.
5. A. Kukol, *Molecular Modelling of Proteins*, 2nd Edition, Springer, 2015.

THIRD YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - III, SEMESTER - V

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Organometallic Chemistry	CY-301	3-1-4	06	100	25	60	40	225
2.	Pericyclic Reactions and Photochemistry	CY-303	3-1-4	06	100	25	60	40	225
3.	Analytical Chemistry	CY-305	3-0-4	05	100	00	60	40	200
4.	Unit Process in Organic Chemistry Industries	CY-307	3-0-0	03	100	00	00	00	100
5.	Institute Elective-1	-	3-0-0	03	100	00	00	00	100
Total contact hours per week=29			**Total Credits=23**				**Total Marks=850**		

THIRD YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - III, SEMESTER - VI

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Interpretative Molecular Spectroscopy	CY-302	3-1-4	06	100	25	60	40	225
2.	Molecules in Motion and Reaction Dynamics	CY-304	3-1-4	06	100	25	60	40	225
3.	Polymer Chemistry	CY-306	3-0-4	05	100	00	60	40	200
4.	Chemistry in Industries	CY-308	3-0-0	03	100	00	00	00	100
5.	Institute Elective-2	-	3-0-0	03	100	00	00	00	100
Total contact hours per week=29			**Total Credits=23**				**Total Marks=850**		

ORGANOMETALLIC CHEMISTRY

CY301

L	T	P	C
3	1	4	6

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain on fundamental principles of organ transition-metal chemistry.
CO2	Discuss the stability and reactivity of organometallic complexes.
CO3	Express into the use of modern methods to characterize organometallic compounds.
CO4	Distinguish between metal carbonyls, cages and rings.
CO5	Explore the applications of organometallics in catalysis.

2. Syllabus:

- **METALLOORGANIC CHEMISTRY-I** **(12 Hours)**
  Introduction, classification based on the nature of metal carbon bond including л-metal complexes, hapticity (η), general methods of preparations and properties, organometallic compounds of alkali metals, Be, Mg, Al, metal olefin complexes; Cyclopentadienyl complexes: Metallocenes, some properties of ferrocene, structure, bonding and reactions in ferrocene molecule, Ionic cyclopentadienyl compounds.

- **METALLOORGANIC CHEMISTRY-II** **(12 Hours)**
  Organometallic compounds: metal alkyls, metal aryls, electron deficient organometallic compounds, electron rich organometallics, Agostic interaction, stereochemicalnonrigidity and fluxional behaviour of organometallic compounds with typical examples, transition metal π complexes with unsaturated organic ligands, fluxional organometallic compounds: fluxionality and dynamic equilibria in compounds such as η2 olefins, η3 allyl and dienyl complexes, Metal hydrogen and metal halogen exchange reactions, Transmetallation reactions, important reactions of Grignard reagent.

- **METAL CARBONYL AND CLUSTERS** **(12 Hours)**
  Metal carbonyl, structure and bonding in mononuclear metal carbonyls, metal clusters, carbonyl clusters, low nuclearity carbonyl clusters, high nuclearity carbonyl clusters, electron counting scheme, Wade's rules, halide type clusters, chevrel phases, Zintlclusters, metal–metal single and multiple bonds, isolobal analogy, cages and rings.

- **ORGANOMETALLIC COMPOUNDS IN HOMOGENEOUS CATALYSIS** **(06 Hours)**
  Homogeneous catalysis: hydrogenation, hydroformylation and polymerization of olefins (Ziegler-Natta catalysis, metallocenes), Mechanism of homogeneous catalysis reactions – addition, elimination, migration and insertion reactions. Wacker's oxidation (Pd-catalyzed), Water gas shift reactions and Fischer-Tropsch process.

(Total Lecture Hours: 42)

3. Practicals:

Identification of cations and simple anions in a mixture of salts containing four/six ions (cations and anions):

Cations : Pb^{2+}, Bi^{3+}, Cu^{2+}, Cd^{2+}, As^{3+}, Sb^{3+}, Sn^{2+} or Sn^{4+}, Fe^{2+}or Fe^{3+}, Al^{3+}, Cr^{3+},Co^{2+}, Ni^{2+}, Zn^{2+}, Mn^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}, NH^{4+} and K^{+}.

Anions : CO_3^{2-}, SO_3^{2-}, CO_2^{3}, SO_2^{-3}, S^{2-}, NO^{-2}, CH_3COO^{-}, NO^{-3}, Cl^{-}, Br^{-}, I^{-}, SO_4^{2-}, PO_4^{3-}, BO_3^{3-}, F^{-} and $C_2O_2^{-4}$.

4. Books Recommended:

1. M. Bochmann, *Oxford Premier Series on Organometallics* Volume 1 & 2, 1st Edition, Oxford Press, Oxford, 2002.
2. A. F. Hill, *Organotransition Metal Chemistry*, The Royal Society of Chemistry, Cambridge, 2002.
3. R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 6th Edition, John Wiley & Sons, New York, 2014.
4. W. W. Porterfield, *Inorganic Chemistry: A Unified Approach*, 2nd Edition, Academic Press, Cambridge, 1993.
5. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, *Inorganic Chemistry-Principles of Structure and Reactivity*, 4th Edition, Pearson Education, London, 2006.

PERICYCLIC REACTIONS AND PHOTOCHEMISTRY

L	T	P	C
3	1	4	6

Scheme

CY303

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Recognize molecular orbital symmetry and Frontier molecular orbitals approach.
CO2	Acquire the knowledge on the laws of photochemistry in various photochemical reactions.
CO3	Illustrate the mechanisms of free radical reactions.
CO4	Formulate molecular structure by using valence bond and molecular orbital theories.
CO5	Explain organic reaction mechanisms for synthesis of bioactive compounds.

2. Syllabus:

- **PERICYCLIC REACTIONS** **(08 Hours)**

  Molecular orbital symmetry, Frontier molecular orbitals approach, 1,3-butadiene, 1,3,5-hexatriene. Classification of pericyclic reactions, FMO and PMO approach, correlation diagrams, Woodward-Hoffman rules, Electrocyclic reactions-conrotatory and disrotatory motions, 4n and 4n+2 systems, Cycloadditions-antrafacial and suprafacial additions in 4n and 4n+2 systems. Sigmatropic rearrangements-suprafacial and antrafacial shifts of H.

- **PHOTOCHEMISTRY** **(15 Hours)**

  Quantum yields, techniques in photochemistry, photosensitization and quenching mechanism. Laws of photochemistry, thermal and photochemical reactions. Photochemistry of olefins: cis-trans isomerisation, dimerisation reactions, Di-π methane rearrangement, Photochemistry of aromatic compounds and its isomerisation.

  Photochemistry of carbonyl compounds: Representation of excited states of ketones, Reactivity of electrically excited ketones, Photo reduction, Norrish type I & II reactions, Reactions of cyclic ketones, oxetane formation (Paterno-Buchi reaction). Photochemistry of aromatic compunds and nitrogen containing organic compounds. Reaction of singlet-oxygen and photocatalytic oxygenation reactions.

- **FREE RADICAL REACTIONS** **(10 Hours)**

  Generation of free radicals - thermolysis, photolysis, redox methods, abstraction, addition and fragmentation; Generation of radical intermediates and its (a) addition to alkenes, alkynes (inter- and intra- molecular) for C-C bond formation and Baldwin's rules (b) fragmentation and rearrangements. Barton deoxygenation and decarboxylation, McMurry coupling. Electron transfer catalysis; Factors influencing radical reactivities- radical stability, polar influences, solvent and steric effects on radical reactions.

- **REAGENTS** **(09 Hours)**

  Mechanism of action, selectivity and utility of following reagents: Selenium dioxide, Aluminium isopropoxide, Diazomethane, Lead tetra acetate, Sodamide, N-Bromosuccinimide, Lithium aluminium hydride, Osmium tetraoxide, Raney nickel, Sodium borohydride, Manganese dioxide, Lithium diisopropylamide (LDA), DCC, DDQ, HIO_4.

(Total Lecture Hours: 42)

3. Practicals:

1. Separation and identification of organic components in binary mixture (Four Mixture).
2. Separation and Identification of organic components in ternary mixture (Four Mixture).

4. Books Recommended:

1. N. J. Turro, *Modern Molecular Photochemistry*, University Science Books, Sausalito, California, 1991.
2. A. Gilbert, J. Baggot, *Essentials of Molecular Photochemistry*, Blackwell Scientific Publications, Oxford & Boston, 1990.
3. I. Fleming, *Pericylic Reactions*, 2nd Edition, Oxford University Press, Oxford, 1998.
4. T. L. Gilchrist, R. C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edition, Cambridge University Press, London, 1979.
5. H. Maskill (Ed.), *The Investigations of Organic Reactions and Their Mechanisms*, 1st Edition, Blackwell Publishing Ltd. Oxford, 2006.

5. Additional Reading Material:

1. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5th Edition, Longman Scientific & Technical, England, 2005.
2. F. A. Carey, R. J. Sundburg, *Advance Organic Chemistry: Structure and Mechanism (Part A) (English)*, 5th Edition, Springer, 2007.

ANALYTICAL CHEMISTRY

L	T	P	C
3	0	4	5

Scheme

CY305

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Gain the basics of Numerical Analysis of analytical data.
CO2	Design the quantitative approaches through conventional methods of analysis.
CO3	Acquire knowledge on electrophoresis and its applications in multidisciplinary areas.
CO4	Develop the basic concepts and applications of atomic spectrometry.
CO5	Establish the correlation between conventional and modern approach for quantitative analysis.

2. Syllabus:

- **NUMERICAL ANALYSIS** **(08 Hours)**

  Presentation of analytical data: accuracy, precision, sensitivity, selectivity, robustness and ruggedness. Classification of errors, significant figures, mean deviation and standard deviations, gaussian distribution, treatment of small sets of data: range rejection of data - 2.5d rule, 4d rule and Q –test.

- **CONVENTIONAL METHODS FOR QUANTITATIVE ANALYSIS** **(14 Hours)**

  Precipitation methods, purity and optimum conditions for precipitation, precipitation from homogeneous solution, washing and ignition of the precipitate, role of organic precipitants in gravimetric analysis. Importance, classification of volumetric methods, acid-base titrations, acid-base titration curves, acid-base indicators, mixed and fluorescent indicators.

  Theory of redox titration curves, oxidizing agents as titrants, applications of iodine as a redox reagent, redox indicators, detection of end point in redox titrations. Theory of precipitation, titration curves, factors influencing solubility of precipitate, titration by turbidity without an indicator, Volhard"s and Mohr"s Methods, adsorption indicators in precipitation titrations. EDTA and complexones, complexometric titration curves, metallochromic indicators, kinetics and selectivity in complexometric titration, typical EDTA titrations, advantages of complexometric titrations.

- **ELECTROPHORESIS** **(08 Hours)**

  Introduction – migration rates and plate hights in CE – electroosmotic flow - various types of electrophoresis -instrumentation – detectors – microchip electrophoresis – CE-MS - applications.

- **ATOMIC SPECTROMETRY** **(12 Hours)**

  Flame spectrometry: introduction, elementary theory, instrumentation, type of burners, interferences, type of interferences, background correction method and applications.

  Atomic Absorption Spectrometry (AAS): Principle, instrumentation, production of atoms and ions, burners, detectors, advantage and disadvantage of AAS, standard addition method, internal standard method. Atomic Emission Spectrometry (AES): Principle, instrumentation, qualitative and quantitative analysis with AES, plasma emission spectrometry, direct current plasma, inductively coupled plasma, ICP-AES, high energy sources (plasma, arc, and spark), sample introduction and measurements.

(Total Lecture Hours: 42)

3. Practicals:

1. Gravimetric Determination of Calcium as $CaC_2O_4.H_2O$
2. Statistical Evaluation of Acid-Base Indicators.
3. Spectrophotometric Determination of Iron in Vitamin Tablets.
4. Spectrophotometric Measurement of an Equilibrium Constant.
5. Spectrophotometric Analysis of a Mixture: Caffeine and Benzoic Acid in Soft Drink
6. Measuring Manganese in Steel by Atomic Absorption Using a Calibration Curve.
7. Anion Content of Drinking Water by Capillary Electrophoresis.

4. Books Recommended:

1. S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, 3rd Edition, New Academic Science, New Delhi, 2008.
2. D. A. Skoog, D. M. West, Holler, Crouch, *Fundamentals of Analytical Chemistry*, 8th Edition, Cengage Learning, USA, 2013.
3. J. H. Kennedy, *Analytical Chemistry: Principles*, 2nd Edition, Saunders College Publishers, Philadelphia, 1990.
4. G. D. Christian, P. K. Dasgupta, K.A. Schug, *Analytical Chemistry*, 7th Edition, John Wiley & Sons, New York, 2004.
5. R. A. Day, A.L. Underwood, *Quantitative Analysis*, 6th Edition, Prentice Hall, Inc. New Delhi, 1993.

5. Additional Reading Material:

1. R. M. Verma, *Analytical Chemistry: Theory and Practice*, 3rd Edition, CBS Publishers, New Delhi, 2004.
2. H. Kaur, *Instrumental Methods of Chemical Analysis (Analytical Chemistry)*, Pragati Prakashan, Meerut, 2012.

UNIT PROCESS IN ORGANIC CHEMISTRY INDUSTRY

L	T	P	C
3	0	0	3

Scheme

CY307

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Acquire an introductory knowledge of chemical industry and unit processes.
CO2	Build a bridge between theoretical and practical concept used in industry.
CO3	Explore the various synthetic methods of producing industrial chemicals and their applications.
CO4	Apply knowledge about the basic chemistry of production.
CO5	Appraise the industrial chemical process of transforming raw materials to desired products.

2. Syllabus:

- **NITRATION** **(06 Hours)**
  Introduction, Nitrating Agents, Aromatic Nitration, Process Equipment for Technical Nitration, Batch Nitration, Continuous Nitration, manufacturing of nitrobenzene by batch and continuous process using fortified spent acid, m-dinitrobenzene and p-nitro acetanilide.

- **AMINATION BY REDUCTION & AMMONOLYSIS AND HALOGENATION** **(08 Hours)**
  Amination: Introduction, Different types of reduction reactions, Schimdt and Biazzi nitrators, different reduced products of nitrobenzene, manufacturing of aniline by Bechamp reduction, m-nitro aniline and aniline by ammonolysis.
  Halogenation: Introduction, different halogenating agents and halogenation reactions, mechanism and manufacturing of BHC and chlorobenzene.

- **SULFONATION & SULFATION** **(05 Hours)**
  Introduction, Sulfonating & Sulfating agents, Sulfonation of Aromatic Compounds. Chemical and physical factors in sulfonation and sulfation, Commercial manufacturing of benzene sulfonic acid (Barbet process) and naphthalene sulfonic acid.

- **OXIDATION** **(06 Hours)**
  Introduction, Types of oxidizing agents and reactions, Oxidation of toluene with MnO_2. Manufacture of acetaldehyde from acetic acid and acetic acid from ethanol. Commercial manufacturing of benzoic acid and phthalic anhydride.

- **HYDROGENATION** **(5 Hours)**
  Introduction and scope, properties and sources of hydrogen, gas catalytic hydrogenation and hydrogenolysis, factors affecting hydrogenation, industrial hydrogenation of fat and oil, manufacture methanol from CO_2 and H_2.

- **ALKYLATION** **(05 Hours)**
  Introduction, Types of alkylation, alkylating agents, factors controlling alkylation, equipment for alkylation, manufacture of alkyl aryl sulphonates and ethylbenzene by continuous process.

- **ESTERIFICATION AND HYDROLYSIS** **(07 Hours)**
  Esterification: Introduction, Esterification of organic acids. Commercial manufacture of some important compounds.

Hydrolysis: Introduction, Hydrolysing agents, Equipment for hydrolysis, industrial hydrolysis of fat, manufacture of ethanol from ethylene (Shell process) and phenol from benzene sulfonic acid.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. P. H. Groggins, *Unit Processing of Organic Synthesis*, 5th Edition, Tata-McGraw Hill, New Delhi, 2001.
2. C. E. Dryden, M. Gopalarao (Ed.), M. Sitting (Ed.), *Dryden's Outlines of Chemical Technology*, 2nd Edition, East-West Pub., New Delhi, 1997.
3. R. N. Shreve, G. T. Austin, *Shreve's Chemical Process Industries*, 5th Edition, McGraw-Hill Pub., New York, 1984.
4. R. M. Felder, R. W. Rousseau, *Elementary Principles of Chemical Processes*, 3rd Edition, John Wiley, New York, 2000.
5. J. A. Kent (Ed.) *Riegel's Handbook of Industrial Chemistry*, 10th Edition, Kluwer Academic / Plenum Publishers, New York, 1985.

THIRD YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - III, SEMESTER - VI

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Interpretative Molecular Spectroscopy	CY-302	3-1-4	06	100	25	60	40	225
2.	Molecules in Motion and Reaction Dynamics	CY-304	3-1-4	06	100	25	60	40	225
3.	Polymer Chemistry	CY-306	3-0-4	05	100	00	60	40	200
4.	Chemistry in Industries	CY-308	3-0-0	03	100	00	00	00	100
5.	Institute Elective-2	-	3-0-0	03	100	00	00	00	100
Total contact hours per week=29			**Total Credits=23**			**Total Marks=850**			

INTERPRETATIVE MOLECULAR SPECTROSCOPY

L	T	P	C
3	1	4	6

Scheme

CY302

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain the theories and basic principles of spectroscopic techniques.
CO2	Acquire the effect of solvent and hydrogen bonding on vibrational frequencies.
CO3	Identify the organic functional groups by FT-IR.
CO4	Enumerate gas-phase reactions and to predict the fragmentation of organic molecules by mass spectrometry.
CO5	Elucidate an unknown structure, or to solve a structure-related problem by utilizing spectroscopic data.

2. Syllabus:

- **UV-VISIBLE ABSORPTION AND EMISSION SPECTROSCOPY** **(10 Hours)**

Mechanism of absorption and emission of radiation by organic compounds, shape of absorption and emission bands and Franck-Condon principle. Various electronic transitions, Lambert-Beer law, effect of solvent on electronic transition, Ultraviolet bands for carbonyl compound, unsaturated carbonyl compounds, Woodward-Fiese's rules for conjugated dienes and carbonyl compounds, UV spectra of aromatic and heterocyclic compounds steric effect in biphenyls. Principles, origin of fluorescence and phosphorescence spectra, variables affecting fluorescence and phosphorescence spectra, instrumentation and applications. Delayed fluorescence, determination of fluorescence quantum yield, introductory Time-resolved fluorescence spectroscopy, types of relaxation processes.

- **INFRARED SPECTROSCOPY** **(07 Hours)**

Instrumentation and sample handling, characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines, carbonyl compounds, esters, amides, anhydrides, lactones and lactams. Effect of solvent and hydrogen bonding on vibrational frequencies, overtones, IR of gaseous, solids and polymeric materials.

- **NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY** **(15 Hours)**

NMR phenomenon, spin ½ nuclei, (1H, 13C, 31P and 19F), Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift δ, inductive and anisotropic effects on δ, chemical structure correlations of δ, chemical and magnetic equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns, second order effects, examples of AB, AX and ABX systems, simplification of second order spectrum, selective decoupling, use of chemical shift reagents for stereochemical assignments. 13C NMR, introduction to FT technique, relaxation phenomena, NOE effects, 1H and 13C chemical shifts to structure correlations.

- **MASS SPECTROMETRY** **(10 Hours)**

Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution

MS, soft ionization methods, ESI-MS and MALDI-MS, illustrative examples from macromolecules and supramolecules, Fragment ions of odd and even electron types – rearrangement ions – factors affecting cleavage patterns –simple and multicentre fragmentation – McLafferty rearrangement – Retro Diels-Alder fragmentation. Mass spectra of hydrocarbons, alcohols, phenols, aldehydes, ketones, carboxylic acids, amines and their derivatives. Studies of inorganic / coordination and organometallic representative compounds.

(Total Lecture Hours: 42)

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3. Practicals:

1. UV-visible spectrometric determination of iron content in tablets OR nicotine content in cigarette tobacco.
2. UV-visible spectrometric determination of the concentration of KMnO4 and K2Cr2O7.
3. Kinetics of Hydrolysis of Acetic Anhydride by In-Situ FTIR Spectroscopy
4. Analysis of drugs (PCM, Crocin, Aspirin, Ibuprofen) from provided samples & determine using FTIR spectroscopy.
5. Determination of caffeine content in coffee using Fourier transform infra-red spectroscopy in combination with attenuated total reflectance technique.
6. Determination of acid dissociation constant by ^{1}H-NMR spectroscopy.
7. Measuring alcohol content in cough syrup using ^{1}H-NMR spectroscopy.
8. Synthesis of Aspirin and characterization of its purity by FTIR and 1H-NMR.

3. Books Recommended:

1. K. W. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce, *Spectrometric Identification of Organic Compounds*, 8th Edition, John Wiley & Sons, New York, 2014.
2. J. R. Lakowicz, *Principles of Fluorescence Spectroscopy*, 3rd Edition, Springer, USA, 2006.
3. M. Sauer, J. Hofkens, J. Enderlein, *Basic Principles of Fluorescence Spectroscopy*, Wiley-VCH, New York, 2011.
4. J. H. Gross, *Mass Spectrometry*, 2nd Edition, Springer Berlin Heidelberg, Germany, 2011.
5. G. M. Lampman, D. L. Pavia, G. S. Kria, J. R. Vyvyan, *Spectroscopy International Edition*, 4th Edition, Cengage Learning India Pvt. Ltd., New Delhi, 2012.

MOLECULES IN MOTION AND REACTION DYNAMICS

L	T	P	C
3	1	4	6

Scheme

CY304

1. Course Outcomes (Cos):

At the end of the course students will be able to:

CO1	Interpret rate of reactions through various kinetic theories and understand mechanism of enzyme catalysis.
CO2	Explain the advances in electrodes and electrolytic reactions.
CO3	Demonstrate the deep theoretical knowledge of colloidal chemistry.
CO4	Accumulate the theoretical basics of statistical thermodynamics
CO5	Perform the experiments related to physical chemistry approach which includes Kinetics, Conductometry, Colorimetry, pH-metry, Potentiometry and Titration.

2. Syllabus:

- **CHEMICAL KINETICS - II** **(12 Hours)**

Collision theory, Arrhenius equation, rate determining step (RDS), activation energy concept, transition state theory, steady state and equilibrium approximation, parallel and consecutive reactions, reversible reactions. Temperature dependence and the Arrhenius theory of reaction rates, Collision theory of bi-molecular gaseous reaction, collision and the steric effects, limitations, The transition-state theory, statistical mechanical approach to the transition state theory; derivation of rate equation, Thermodynamic formulation of transition state theory, Unimolecular gas reactions: Lindeman-Christiansen hypothesis, the Hinshelwood's theory, Rice-Ramsperger-Kassel theory. Mechanism and Kinetics of Enzyme catalysis and Surface Reactions. Numericals.

- **ELECTROCHEMISTRY-III** **(12 Hours)**

Different types of electrodes and electrolyte concentration cell, liquid junction potential (LJP), methods for elimination of LJP, salt bridge, concentration cell with and without transference (with derivation of equation for EMF of cell and LJP). Electrode-electrolyte interface and its mechanism of charge transfer. Electrolytic polarization, Decomposition potential, over voltage, concentration polarization, Measurement of over voltage, influence of current density and temperature on over voltage, Ionic discharge as the slow process at cathodes. Tafel and proton transfer theory of hydrogen and oxygen over voltage, applications of EMF in the determination of: solubility product and solubility of sparingly soluble salts, ionic product of water by galvanic cell, transport number of ions, equilibrium constant, pH by hydrogen, glass and quinhydrone electrodes. Numericals.

- **COLLOIDAL CHEMISTRY – II** **(08 Hours)**

Donnan membrane equilibrium, Qualitative understanding of electro-kinetic phenomenon: Electrokinetic phenomena, Electrophoresis, Electro osmosis, Sedimentation potential and streaming potential. Electrical double layer (Stern and DLVO theory), Zeta potential, Mechanism of coagulation, Schulze-Hardy rule, Gold number. Dialysis, electro-dialysis, Ultrafiltration, Ultramicroscope, Charge on colloidal particles, Coagulation of colloidal solution, Flocculation values, Determination of size and colloidal particles. Applications.

- **STATISTICAL THERMODYNAMICS** **(10 Hours)**

Limitations of Classical thermodynamics, Distribution laws: Boltzmann, Bose-Einstein, and Fermi-Dirac, limitations of applicability of various distribution laws. Partition function and its

significance. Translational, rotational, vibrational, and electronic partition functions of diatomic molecules and their evaluation. Relation between partition and their thermodynamic function, average internal energy, heat capacity, Helmholtz free energy and entropy of mono- and di-atomic molecules, Sekur-Tetrode equation. Numericals.

(Total Lecture Hours: 42)

3. Practicals:

1. Determine the order and rate constant of the reaction between $K_2S_2O_8$ and KI. Also study the influence of ionic strength on the rate constant.
2. Study of the effect of substituent on the dissociation constant of weak acid by conductance (Acetic acid, mono-, di-, and tri-chloro acetic acid).
3. Determine the dissociation constants (pK_a values) of tribasic acid by pH-metry (e.g. ortho Phosphoric acid).
4. Preparation of Phenol-Formaldehyde (PF) resin.
5. To determine the solubility product of $BaSO_4$ conductometrically.
6. Study the phase diagram of a binary system (Phenol + water) and the effect of impurities (e.g. NaCl).
7. Verify the Onsager equation using KCl, K_2SO_4 and $BaCl_2$ as electrolytes and determine their equivalent conductivity at different dilutions and from them find out the equivalent conductivity of a weak electrolyte at infinite dilution.
8. To determine the CMC of any surfactant at room temperature in aqueous solution by conductance method.

4. Books Recommended:

1. S. Glasstone, *Thermodynamics for Chemists*, 1st Edition, Affiliated East-West Press Pvt. Ltd., New Delhi, 2009.
2. R. P. Rastogi, R. R. Misra, *An Introduction to Chemical Thermodynamics*, 4th Edition, Vikas Publishing House Pvt. Ltd., New Delhi, 1986.
3. B. R. Puri, L. R. Sharma, *Principles of Physical Chemistry*, 8th Edition, Vishal Publications, New Delhi, India, 2001.
4. S. Maity, N. Ghosh, *Physical Chemistry Practical*, 1st Edition, New Central Book Agency (P) Ltd., India, 2012.
5. M. C. Gupta, *Statistical Thermodynamics*, 2nd Edition, New Age International Pvt. Ltd., 1995.

POLYMER CHEMISTRY

L	T	P	C
3	0	4	5

Scheme

CY306

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain the general reaction course and reaction mechanism for common polymerizations.
CO2	Describe and compare the polymerization principles.
CO3	Calculate parameters and outcomes of polymerizations.
CO4	Evaluate polymerizations from a green chemistry perspective.
CO5	Practically perform different types of polymerizations.

2. Syllabus:

- **INTRODUCTION** **(04 Hours)**

  Introduction, classification of polymers, general characteristics of polymers in comparison with organic compound, distinction between plastics, elastomers, fibres and liquid resins, properties of polymers.

- **CHAIN POLYMERIZATION** **(10 Hours)**

  Preparative methods, properties and application: Low density (branched) polyethylene, polypropylene, high density (linear), polyethylene, polypropylene, natural rubber, rubbers derived from butadiene–acrylic acid copolymers, stereo-regular polybutadienes, polychloroprene (neoprene), styrene- butadiene –acrylonitrile copolymers.

  Carbon–carbon polymers- polystyrene, copolymers of polystyrene, acrylic polymers–acrylic fibers, acrylic adhesives, poly acrylates, polymethyl methacrylate(PMMA), polyvinyl acetate (PVA), polyvinyl alcohol, poly vinylchloride, fluorocarbon polymers.

- **CONDENSATION POLYMERIZATION** **(10 Hours)**

  Preparative methods, properties and application: Polyamides, Nylon 6, Nylon 66, Nylon 610, polyesters, polyether and related polymers – poly ethylene terephthalate (PET), polybutyllene, terphthalate (PBT), aromatic polyesters, polycarbonate, polyurethanes – Flexible and rigid polyurethane, polyurethane elastomers, coatings, adhesives, sulphur, containing polymers. Thermosetting resins – phenolic resins, amino resins epoxy resins.

- **POLYMER PROCESSING** **(06 Hours)**

  Basic processing operations, extrusion, calendaring, sheet forming, stamping, casting, fibre spinning, injection moulding, thermoforming, vulcanisation of elastomers.

- **POLYMER CHARACTERIZATION** **(12 Hours)**

  Identification and characterization of polymers: tensile strength, impact strength, elongation at break, water resistance, hardness, heat distortion temperature, brittleness, flexural strength, molecular weight and molecular weight distribution-number, weight and viscosity average molecular weights of polymers, methods of determining, molecular weight, Rheology of polymer, Fractionation of polymers, chemical analysis of polymers, mechanical properties of polymers glassy state, glass transition temperature, factor's affecting glass transition temperature, degradation of polymers by thermal, oxidative, mechanical and chemical methods.

(Total Lecture Hours: 42)

3. Practicals:

1. To study synthesis of Polyester resin.
2. To study synthesis of Polyurethane resin.
3. To study synthesis of acrylic polymer.
4. To study synthesis of poly styrene by emulsion polymerization.
5. To study synthesis of poly styrene by suspension polymerization.
6. To perform FTIR analysis of synthesized polymers.
7. To perform TGA/DSC analysis of synthesized polymers.
8. To prepare composite from Unsaturated Polyester Resin using Jute / Glass fiber as reinforcing material.

4. Books Recommended:

1. F. W. Billmeyer, *Textbook of Polymer Science*, 3rd Edition, Wiley-Interscience, 2007.
2. D. D. Deshpande, *Physical Chemistry of Macromolecules*, Vishal Publications, New Delhi, 1985.
3. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, *Polymer Science*, Wiley Eastern Ltd., 1986.
4. V. K. Ahluwalia, Anuradha Mishra, *Polymer Science: A Textbook*, 1st Edition, CRC Press, 2008.
5. R. Seymour, *Introduction to Polymer Chemistry*, Wiley-Interscience, 1981.

5. Additional Reading Material:

1. P. J. Flory, *Principles of Polymer Chemistry*, 1st Edition, Cornell University Press, 1953.
2. G. Odian, *Principles of Polymerization*, 4th Edition, Wiley – Interscience, 2004.
3. K. J. Saunders, *Organic Polymer Chemistry*, 2nd Edition, Chapman and Hall, London, 1973.
4. R. B. Seymour, G. S. Kirshenbaum, *High Performance Polymer: Their Origin and Development*, 1st Edition, Elsevier, 1986.
5. P. W. Morgen, *Condensation Polymers by Interfacial and Solution Methods*, 1st Edition, Interscience publishers, New York 1965.

CHEMISTRY IN INDUSTRIES

L	T	P	C
3	0	0	3

Scheme

CY308

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain process technologies of various organic and inorganic process industries.
CO2	Prepare the process flow diagram and various process parameters.
CO3	Explore various synthetic methods of producing industrial chemicals, their applications.
CO4	Recognize the basic chemistry of production.
CO5	Acquire knowledge about laboratory and plant safety and management.

2. Syllabus:

- **NITROGEN INDUSTRY** **(05 Hours)**
  Introduction, manufacture of synthetic nitrogen products and miscellaneous chemicals such as ammonia, hydro amine, fluorocarbon and various types of nitrogenous fertilizers such as urea, ammonium sulphate, ammonium nitrate, calcium ammonium nitrate.

- **FERMENTATION INDUSTRY** **(05 hours)**
  Introduction, culture development, inoculum preparation, nutrients for microorganisms, toxic effects on culture, manufacture of industrial alcohol, absolute alcohol, vinegar, downstream processing.

- **PERFUMERY INDUSTRY** **(05 hours)**
  Compounds used for different perfumes, essential oils, preparation of phenyl ethanol, Yara-Yara, musk ketone, musk xylene, benzyl acetate, synthetic musk, jasmine.

- **AGROCHEMICAL AND PESTICIDE INDUSTRY** **(05 Hours)**
  Classification of agrochemicals, classification of insecticide, ammonium phosphate, super phosphate, BHC, Uses of agrochemicals and environments.

- **INDUSTRIAL GASES** **(05 Hours)**
  Industrial Gases – Manufacture of hydrogen, oxygen, nitrogen, carbon dioxide and sulphur dioxide.

- **LABORATORY SAFETY AND PROCESS SAFETY** **(06 Hours)**
  Personal protective equipment, nature of the hazard and the task, compatibility with other PPE, chemicals being used, including concentration and quantity, hazards posed by the chemicals, routes of exposure for the chemicals, material the PPE is constructed of, safety signs, hazard assessment.

- **QUALITY MAAGEMENT TOOLS AND METHODS** **(05 Hours)**
  Flow Chart, histogram, cause-and-effect diagram, check sheet, scatter diagram, control charts, pareto charts.

- **BASIC CHEMICAL ENGINEERING CONCPT FOR CHEMISTS** **(06 Hours)**
  Initial design steps – identifying a process route, basic conceptual process design and flow-sheeting, Mass and energy balances, reactor design, separation processes, process control, scale-up/ commercialization.

(Total Lecture Hours: 42)

3. Books Recommended:

1. G. T. Austin, *Shreve's Chemical Process Industries*, 5th Edition, Tata McGraw Hill, 2017.
2. J. P. Agrawal, *High Energy Materials: Propellants, Explosives and Pyrotechnics*, 1st Edition, Wiley-VCH, 2015.
3. B. K. Sharma, *Industrial Chemistry*, 3rd Edition, Krishna Prakashan Media (P) Ltd., Meerut, 2001.
4. M. Ash, I. Ash, *Formulary of Cosmetic Preparations*, 1st Edition, Chemical Publishing, 1977.
5. F. V. Wells, M. Billot, *Perfumery Technology*, 2nd Edition, Longman Higher Education, 1981.

4. Additional Reading Materials:

1. J. A. Kent, *Riegel's Hand Book of Industrial Chemistry*, 6th Edition, CBS Publishers & Distributors, New Delhi, 1986.
2. M. L. Srivastava, *Fermentation Technology*, Narosa Publisher, 2008.

FOURTH YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - IV, SEMESTER - VII

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Advanced Inorganic Chemistry	CY-401	3-1-4	06	100	25	60	40	225
2.	Methods in Organic Synthesis	CY-403	3-1-4	06	100	25	60	40	225
3.	Quantum Chemistry	CY-405	3-1-4	06	100	25	60	40	225
4.	Core Elective-1	CY-4XX	3-0-0	03	100	00	00	00	100
Total contact hours per week=27			**Total Credits=21**			**Total Marks=775**			

Elective-1 (CY-4XX)

Sr. No.	Code	Subject
1.	CY-421	Corrosion Science and Technology
2.	CY-423	Surfactant Chemistry
3.	CY-425	Petrochemicals
4.	CY-427	Chemistry of Nanomaterials

FOURTH YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - IV, SEMESTER - VIII

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Symmetry, Spectra & Magnetism	CY-402	3-1-4	06	100	25	60	40	225
2.	Chemistry of Natural Products	CY-404	3-1-4	06	100	25	60	40	225
3.	Physical Aspects of Molecular spectroscopy	CY-406	3-1-4	06	100	25	60	40	225
4.	Core Elective-2	CY-4YY	3-0-0	03	100	00	00	00	100
Total contact hours per week=27			**Total Credits=21**			**Total Marks=775**			

Elective-2 (CY-4YY)

Sr. No.	Code	Subject
1.	CY-422	Purification and Separation Methods in Chromatography
2.	CY-424	Fluorescence Spectroscopy
3.	CY-426	Polymer and Coating Technology
4.	CY-428	Organic Materials
5.	CY-432	Drugs and Dyes
6.	CY-434	Green Chemical Processing

ADVANCED INORGANIC CHEMISTRY

L	T	P	C
3	1	4	6

CY401 **Scheme**

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explore thermodynamic and kinetic of complex formation in solution.
CO2	Study on reaction mechanisms of complexation in solution.
CO3	Discuss on possible electronic transitions in metal complexes.
CO4	Write photochemical reaction of metal complexes.
CO5	Summarize polymeric inorganic compounds.

2. Syllabus:

- **THERMODYNAMIC AND KINETIC BEHAVIOR OF METAL COMPLEXES (14 Hours)**
  Stability, step wise formation constants and overall formation constants. Kinetic versus Thermodynamic stability, labile and inert octahedral complexes according to valence bond and crystal field theory. factors affecting stability constants, Chelates and macrocyclic effects, Irving Williams order, determination of stability constant by various methods (spectrophotometric and pH-metric), conditional stability constants and their importance in complexometric EDTA titration of metal ions, statistical and non-statistical factors affecting stability of complexes in solution.

- **REACTION MECHANISMS IN TRANSITION METAL COMPLEXES (12 Hours)**
  Substitution reactions in octahedral and square planar complexes, Reaction mechanism of ligand substitution reactions in octahedral complexes: SN_1 (D-process), SN_2 (A-process), solvent intervention, ion pair formation, conjugate base formation SN_1CB. Solvolysis reactions: acid and base hydrolysis, Trans effect, theories of Trans effect, Redox (one and two-electron transfer) reactions, inner sphere and outer sphere processes, Creutz-Traube complexes.

- **INORGANIC PHOTOCHEMISTRY (08 Hours)**
  Introduction of inorganic photochemistry, Photochemically excited states and excited state processes for transition metal complexes, Types of photochemical reactions in transition metal complexes, Ligand-field photochemistry of chromium(III) complexes, Photo substitution reactions, Adamson's rules, photochemistry of Cobalt(III) complexes, Mechanism of photoreduction: photophysics and photochemistry of Ruthenium-polypyridine complexes, Applications of photochemical inorganic reactions in synthesis, Catalysis, Biological processes, chemical actinometer and in laser.

- **POLYMERIC INORGANIC COMPOUNDS (08 Hours)**
  Types of inorganic polymers, comparison with organic polymers, synthesis, structural aspects and applications of silicones and siloxanes. Borazines, silicates and phosphazenes, and polysulphates.

(Total Lecture Hours: 42)

3. Practicals:

Preparation and characterization (UV-Vis, FT-IR, thermal analyses, etc.) of the following complexes:

1. Potassium tris(oxalato)aluminate(III)
2. Potassium tris(oxalaato) chromate(III)
3. Sodium hexa(nitro)cobaltate(III)
4. Hexa(ammine)cobalt(III)
5. Tetrapyridinecopper(II)persulphate
6. Dinitrotetrapyridinenickel(II)
7. Hexamminenickel (II) chloride
8. Bis(acetylacetonato)copper(II)
9. Tris(acetylacetonato)iron(III)
10. Tris(acetylacetonato)manganese(III).

4. Books Recommended:

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, *Inorganic Chemistry - Principles of Structure and Reactivity*, 4th Edition, Pearson Education, 2006.
2. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Blackwell Science, 1996.
3. H. J. Emeleus, A. G. Sharpe, *Modern Aspects of Inorganic Chemistry*, 4th Edition, Routledge & Kegan Paul, London, 1973.
4. W. W. Porterfield, *Inorganic Chemistry: A Unified Approach*, 2nd Edition, Elsevier Publishers, 2005.
5. A. W. Adamson, P. D. Fleschaner, *Concepts of Inorganic Photochemistry*, Wiley, 1975.

5. Additional Reading Material:

1. V. Balzani, Carassiti, *Photochemistry of Coordination Compounds*, Academic press, 1970.

METHODS IN ORGANIC SYNTHESIS

CY403

L	T	P	C
3	1	4	6

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Show the role of protecting groups in organic synthesis.
CO2	Extend the knowledge in the mechanisms of various named reactions and their significance in synthesis of drugs.
CO3	Explain the mechanistic and stereo chemical aspects in the reactions of carbon-carbon and carbon-hetero multiple bonds molecules.
CO4	Illustrate the mechanistic details of various rearrangement reactions in organic molecules.
CO5	Demonstrate drugs discovery, diversity and their classification, and to understand their mode of action.

2. Syllabus:

- **PROTECTING GROUPS** **(03 Hours)**
  Protection and deprotection methodology for functional groups. Synthetic applications in peptide synthesis, biology and medicine.

- **REARRANGEMNTS IN CARBON SKELETON** **(06 Hours)**
  Classification and general mechanistic treatment of nucleophilic, free radical and electrophilic rearrangements, Pinacol-Pinacolone, Semipinacol, Wagner Meerwein, Favorskii Curtius, Hoffmann, Schmidt, Beckmann's, Wittig, Benzil-Benzilic acid, Demjanov, Claisen-Johnson-Ireland and Oxy-Cope rearrangements.

- **REMODELING OF CARBON SKELETON** **(04 Hours)**
  Cleavage of C-C bonds. Decarboxylation, Baeyer-Villiger oxidation, and 1,2-diol cleavage in a total synthesis, synthetic utilization of the double bond cleavage reactions.

- **ASSYMMETRIC SYNTHESIS** **(06 Hours)**
  Stereochemistry of larger rings, fused and bridged rings, synthesis of Taxol and strychnine, Sharpless asymmetric epoxidation, Jacobsen epoxidation, Shi epoxidation. Alkenes to diols, Sharpless asymmetric dihydroxylation, metathesis reactions.

- **ADDTION TO CARBON-CARBON AND CARBON-HETEROATOM MULTIPLE BONDS** **(12 Hours)**
  Mechanistic and stereochemical aspects of additon reactions involving electrophiles, nuclophiles and free radicals, regio- and chemoselectivity, orientation and reactivity, addtion to cyclopropane ring, hydrogenation of double and triple bonds, hydrogenation of aromatic rings, hydroboration, Michael reaction, ene reaction, Wittig reaction, Perkin reaction, Claisen – Schmidt condensation, Peterson's synthesis, Cannizaro and cross Cannizaro reactions, Benzoin condensation, Wolff-Kishner reduction, Clemmenson reduction, MPV reduction, Birch reduction, Riemer-Tiemann reaction, Gattermaan reaction, Chichibabin reaction. Uses of organoboron compounds in organic synthesis. Addition of Grignard reagent, organo zinc, organo copper, and organo lithium reagents to carbonyl and unsaturated carbonyl compounds. Mechanism of considensation reactions involving

enolates- Knoevenagel, Mannich and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

- **DRUGS** **(11 Hours)**

Drug discovery and drug diversity, classification of drugs, chemistry of sulfa drugs, antipyretics and analgesics, antibiotics, antituberculor, antifungal and anti-inflammatory drugs.

(Total Lecture Hours: 42)

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3. Practicals:

1. Backmann's rearrangement. #
2. Synthesis of caprolactum. #
3. Cannizzaro reaction. #
4. Sandmayer's reaction. #
5. Asymmetric synthesis (ketone reduction/epoxidation). #
6. Diazocoupling. #
7. Nitration. #
8. Acetyl salicylicacid from Asprin tablets.
9. Ibuprofen from Ibuprofen tablets

#Identification by spectroscopic methods.

Synthesis of various organic compounds by various chemical approaches.

4. Books Recommended:

1. W. Carruthers, I. Coldham, *Modern Methods of Organic Synthesis*, 4th Edition, Cambridge University, 2005.
2. F. A. Carey, R. J. Sundburg, *Advance Organic Chemistry: Structure and Mechanism (Part A) (English)*, 5th Edition, Springer, 2007.
3. B. Reinhard, *Advance Organic Chemistry: Reaction Mechanisms*, 1st Edition, Elsevier, 2002.
4. G. S. Zweifel, M. H. Nantz, *Modern Organic Synthesis*, 1st Edition, W. H. Freeman, 2006.
5. H. O. House, *Modern Synthetic Reactions*, 2nd Edition, W. A. Benjamin, 1972.

5. Additional Reading Material:

1. R. O. C. Norman, J. M. Coxon, *Principles of Organic Synthesis*, 3rd Edition, Nelson Thornes, 2005.
2. S. Warren, *Designing Organic Syntheses: A programmed Introduction to the Synthon Approach*, John Wiley and Sons, 2009.
3. T. L. Lamke, D. A. Williams, V. F. Roche, S. W. Zito, *Foye's Medicinal Chemistry*, 7th Edition, Lippincott Williams and Wilkin's Publisher, 2012.
4. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5th Edition, Pearson India, 2005.
5. R. K. Bansal, *Laboratory Manual of Organic Chemistry*, 5th Edition, New Age International Pvt. Ltd. Publishers, 2008.

QUANTUM CHEMISTRY

L	T	P	C
3	1	4	6

Scheme

CY405

1. Course Outcomes (Cos):

At the end of the course students will be able to:

CO1	Appraise the fundamentals of classical quantum chemistry.
CO2	Gain basics of various operators with their applications.
CO3	Calculate eigen values and eigen functions for various systems.
CO4	Solve mathematical problems based on quantum mechanics.
CO5	Perform the experiments related to physical chemistry approach which includes Kinetics, Conductometry, Colorimetry, pH-metry, Potentiometry and titration.

2. Syllabus:

- **QUANTUM MECHANICS – I** **(14 Hours)**
  Black body radiation, Classical Theory of Rayleigh-Jean, and Planck's theory, Photoelectric effect, Einstein's Quanta, Compton effect, Dual nature of electromagnetic radiation, de Broglie's hypothesis, Wave particle duality, Matter wave, Concept of wave packets, Uncertainty principle, its various mathematical forms and its justifications.

- **QUANTUM MECHANICS – II** **(14 Hours)**
  Operators, Linear operators, Hermitian operators, Postulates of Quantum Mechanics, Schrödinger wave equation (Time dependent and time independent), Solution of Schrödinger equation as wave function and energy (eigen values and eigen functions), Commutators and their implication with respect to x, px, Expectation values, Properties of eigen functions, Energy quantization for hydrogen atom. Numericals.

- **QUANTUM MECHANICS – III** **(14 Hours)**
  Simple systems: 1-D, 2-D, 3-D box (eigen values, eigen functions, expectation values, quantum numbers, degeneracy, probability density), Simple Harmonic Oscillator: Setting the Schrödinger equation, derivation, eigen values and eigen functions, zero point energy, Basics of hydrogen atom and rigid rotar.

(Total Lecture Hours: 42)

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3. Practicals:

1. Determine the equivalent conductance of weak electrolyte at infinite dilution using Kohlraush law.
2. To determine the concentration of HCl/ H_2SO_4, acetic acid, Copper sulphate in given solution by conductometric titration.
3. To determine the hydrolysis constant of aniline hydrochloride.
4. Potentiometric titration of halide mixture (Chloride, Bromide and Iodide) with standard $AgNO_3$.
5. Determination of the equilibrium constant of the reaction $KI + I_2 = KI_3$ (Partition Coefficient).
6. Polymer synthesis of poly vinyl alcohol (PVA) from poly vinyl acetate (PVAc) and estimate molecular weight from solution viscosity.

7. Determination of dissociation constant pK_{in} of methyl red indicator spectrophotometrically.
8. Preparation of Urea-Formaldehyde (UF) resin.

4. Books Recommended:

1. G. M. Barrow, *Physical Chemistry*, 6th Edition, McGraw-Hill, Kogakusha Ltd., New Delhi, 1973.
2. D. A. Skoog, F. J. Hooes, T. A. Nieman, *Principles of Instrumental Analysis*, 5th Edition, Saunders College Publishing, Philadelphia, 1998.
3. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press Pvt. Ltd., New Delhi, 2009.
4. N. Levine, *Quantum Chemistry*, 4th Edition, Prentice Hall, Englewood Cliffs, New Jersey, 1991.
5. S. Maity, N. Ghosh, *Physical Chemistry Practical*, 1st Edition, New Central Book Agency (P) Ltd., India, 2012.

CORROSION SCIENCE AND TECHNOLOGY

L	T	P	C
3	0	0	3

Scheme

CY421

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain the basics of corrosion.
CO2	Relate to the corrosion principles with its significance.
CO3	Correlate about the proposed corrosion theory with their applications.
CO4	Interpret and correlate various corrosion parameters.
CO5	Collaborate several corrosion control approaches.

2. Syllabus:

- **FUNDAMENTALS OF CORROSION** **(05 Hours)**
  Introduction to Corrosion, its forms and classification, cost of corrosion, environments, corrosion engineering, and future outlook.

- **CORROSION PRINCIPLES** **(10 Hours)**
  Corrosion rate expressions, electrochemical aspects-electrochemical reactions, polarization, passivity, environmental effects- effect of oxygen and oxidizers, effects of velocity, effect of temperature, effects of corrosive concentration, effect of galvanic coupling, metallurgical and other aspects- metallic properties, economic considerations, importance of inspection.

- **MIXED POTENTIAL CORROSION THEORY AND ITS APPLICATIONS** **(12 Hours)**
  Free energy, cell potentials, EMF and galvanic series, exchange current density, activation, concentration and combined polarizations, mixed potential theory, mixed electrodes, passivity, mechanism of the growth and break-down of passive film, predicting corrosion behaviour, effect of oxidizers and velocity, galvanic coupling, alloy evaluation, noble metal alloying, corrosion rate measurements by Tafel extrapolation and linear polarization methods.

- **CORROSION CONTROL** **(15 Hours)**
  Material selection- Selection of proper corrosion resistant metals and alloys for specific environment, metal purification, non-metallics, Alteration of environment- Changing medium, temperature, inhibitors- adsorption type inhibitors, scavengers, oxidizers, vapor-phase inhibitors, Proper design, Cathodic protection- primary protection, secondary protection by impressed current and sacrificial anode methods, selection of anodes, backfills, protective currents, stray current effects and applications, anodic protection- active- passive behavior of materials and structures, heat treatments- annealing, hardening, carburizing, nitriding, potentiostat, electrodes, environments and their comparison, Coatings.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. J. T. N. Atkinson, H. Van Droffelaar, *Corrosion and its Control: An Introduction to the Subject*, 2nd Edition, NACE, Houston, TX, 1995.

2. G. Fontana Mars, *Corrosion Engineering*, 3rd Edition, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2005.
3. J. C. Scully, *The Fundamentals of Corrosion*, 3rd Edition, Pergamon Press, Oxford, UK, 1990.
4. K. R. Trethewey, J. Chamberlain, *Corrosion for Students of Science and Engineering*, 2nd Edition, Longman Scientific and Technical, Harlow, UK, 1996.
5. H. H. Uhlig, R. W. Revie, *Corrosion and Corrosion Control: An Introduction to Corrosion Science and Engineering*, 3rd Edition, John Wiley, New York, 1985.

SURFACTANT CHEMISTRY

CY423

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain the basics of surfactants and their importance in various fields of engineering.
CO2	Appraise a deep knowledge on their phase study and micellization process.
CO3	Correlate the solution behavior surfactants.
CO4	Evaluate various models defining surfactant solutions.
CO5	Collaborate the skill to apply the advances of surfactants.

2. Syllabus:

- **INTRODUCTION** **(07Hours)**
  Molecular structure of surfactants, Classification of surfactants, Properties and other criteria influencing surfactant choice, Surface activity, Surface tension, Interfacial and dynamic surface tension, Reduction of Surface, interfacial and dynamic tension by Surfactants, Efficiency and Effectiveness in surface tension Reduction: Krafft point (KP). Test methods for surface and interfacial tension measurements: Wilhelmy Plate, Pendent Drop, Du Nouy's Ring, Drop Volume (Weight), and Spinning Drop. The Economic Importance of Surfactants, Surfactants in the Environment, Biodegradation of Surfactants.

- **ADSORPTION OF SURFACTANTS** **(07 Hours)**
  Gibbs Monolayers, Surface Pressure, Surface Potential, Surface Rheology, Gibbs Surface Excess, Electrical Double layer, Gibbs Adsorption Isotherm, Equation of State Approach, Classification of Solid–Vapor Adsorption Isotherms: Langmuir, Freundlich, Brunauer–Emmett–Teller (BET) Isotherm for Surface Area calculation.

- **PHASE BEHAVIOR OF SURFACTANT SYSTEMS** **(07 Hours)**
  Solubility-Temperature relationship for Ionic surfactants, surfactant self-assembly, structure of Liquid Crystalline Phases: Hexagonal, Micellar Cubic, Lamellar, Bicontinuous Cubic. Phase Diagrams of Ionic and Nonionic Surfactants.

- **MICELLE FORMATION BY SURFACTANTS** **(07 Hours)**
  The Critical Micelle Concentration (CMC), Packing Parameter, Micellar structure and shape, Aggregation number (N_{agg}), Factors Affecting the CMC in aqueous media: Structure of the Surfactant, the Hydrophobic and Hydrophilic group, the Counterion in Ionic surfactants, Degree of Binding to the Micelle, Electrolyte (inorganic/ organic), and Temperature.

- **SOLUTION PROPERTIES OF SURFACTANTS** **(07 hours)**
  Solubility–Temperature relationship for Surfactants, Thermodynamics of Micellization, Kinetic aspects, Equilibrium aspects, Phase Separation Model, Mass Action Model, Enthalpy and Entropy of Micellization, Driving force for micelle formation, Micellization in Polar and Non-Polar solvents, synergistic or antagonistic micellization in surfactant mixtures (Mixed Micelles). Rheology of surfactant solutions: Introduction to various rheological terms, Rheological behavior of

monomeric solutions and non-interacting micelles, Entanglement networks of rod-like micelles, the rheological behavior of bilayer phases.

- **MULTIDISCIPLINARY APPLICATIONS OF SURFACTANTS** **(07 hours)**
  Surfactants as Foaming and Antifoaming agents, as Dispersants, in Wetting (Contact angle), Spreading and Adhesion, in Nano-emulsions and Microemulsification, in Stabilization of suspensions, in Detergency, in Aerosols, in Personal Care and Cosmetics, in Pharmaceutical Formulations, in Agrochemicals, in the Food Industry.

(Total Lecture Hours: 42)

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3. <u>Books Recommended</u>:

1. T. F. Tadros, *Applied Surfactants - Principles and Applications*, 2nd Edition, Wiley VCH, Verlag GmbH & Co., Germany, 2005.
2. M. R. Porter, *Handbook of Surfactants*, 2nd Edition, Academic and Professional Publishers, 1994.
3. J. Falbe, *Surfactants in Consumer Products Theory, Technology and Applications*, 1st Edition, Springer Verlag, 1987.
4. D. Myers, *Surfaces, Interfaces, and Colloids - Principles and Applications*, 2nd Edition, John Wiley & Sons, Inc., New York, 1999.
5. M. J. Rosen, *Surfactants and Interfacial Phenomena*, 3rd Edition, John Wiley & Sons, Inc., Hoboken, New Jersey, 2004

PETROCHEMICALS

CY425

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Acquire deep knowledge of various theories of petroleum products.
CO2	Demonstrate of the unit processes in manufacture of petrochemicals.
CO3	Explain variety of petrochemical feedstock and products.
CO4	Identify the specifications required for good quality petroleum products.
CO5	Extend the knowledge of the process of purification and fractionation of crude oil.

2. Syllabus:

- **THEORIES OF PETROLEUM PRODUCTS** **(07 Hours)**
  Theories of petroleum formation, composition of petroleum, refining and rectification process of petroleum, light petroleum products – their specification and test methods, cracking and reforming process, reaction taking place in cracking, cracking catalyst, cracking plants.

- **DISTILLATION OF CRUDE PETROLEUM** **(07 Hours)**
  Preparation of petroleum for processing, destruction of petroleum emulsion, electrical desalting plants, methods of petroleum distillation, distillation of crude petroleum, treatment of residual liquid, processing of liquid fuel for petroleum and petroleum products.

- **FRACTIONATION OF PETROLEUM** **(08 Hours)**
  Chemicals derived from C1, C2, C3 and C4 fractions, separation of components of petroleum by using techniques like- compression, absorption, adsorption, low temperature distillation, special and combined techniques. Manufacture of HCN, CS2, Maleic anhydride, Caprolactum and Phthalic anhydride.

- **MANUFACTURE OF PETROCHEMICALS BY FOLLOWING UNIT PROCESS** **(08 Hours)**
  Alkylation: ethyl benzene and isopropyl benzene from benzene. Dehydrogenation: butadiene from butane/butane. Hydration: acetaldehyde from acetylene. Hydrolysis: ethanol from ethylene. Esterification: commercial manufacturing of vinyl acetate. Oxidation: ethylene oxide from ethylene and phenol from cumene Hydroformylation: propionaldehyde from ethylene and synthesis gas.

- **PURIFICATION OF PETROLEUM PRODUCTS** **(06 Hours)**
  Absorptive and adsorptive purification, sulphuric acid purification, alkaline purification, hydrofining, purification in DC electric field-demercaptanisation, stabilisation.

- **PETROLEUM AROMATICS** **(06 Hours)**
  Occurrence, Benzene derivatives, production of aniline, products from toluene, cholorotoluene, sulphonation of toluene, oxidation product of toluene, chemicals from xylene.

(Total Lecture Hours: 42)

3. Books Recommended:

1. S. Matar, L. F. Hatch, *Chemistry of Petrochemical Processes*, 2nd Edition, Gulf Professional Publishing, 2001.
2. J. G. Speight, *The Chemistry and Technology of Petroleum*, 5th Edition, CRC Press, 2014.
3. B. K. Rao, *Modern Petroleum Refining Process*, 2nd Edition, Oxford & IBH Publishing Co. Pvt. Ltd., New Delhi, 1990.
4. B. K. Rao, *A Textbook on Petrochemicals*, 5th Edition, Khanna Publishers, New Delhi, 2010.
5. T. A. George, *Shreve's Chemical Process Industries*, 5th Edition, McGraw-Hill International Edition, 1985.

CHEMISTRY OF NANOMATERIALS

CY427

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Adapt synthetic procedure for processing of nanomaterials as per needs and specifications.
CO2	Acquire knowledge about the electronic, mechanical and thermal properties of nanomaterials.
CO3	Illustrate the structure and morphology of nanomaterials.
CO4	Know the applications of nanomaterials in sustainable developments and technology.
CO5	Extend the knowledge on the synthetic routes for synthesis of nanomaterials

2. Syllabus:

- **STRUCTURES &CLASSIFICATION OF NANOMATERIALS** **(10 Hours)**

  Definition of Nano, Atomic Structure and atomic size, emergence and challenges of nanoscience and nanotechnology, carbon age-new form of carbon (CNT to Graphene), influence of nano over micro/macro, size effects and crystals, large surface to volume ration, surface effects on the properties.

  Types of nanostructure and properties of nanomaterials: One dimensional, Two dimensional and Three dimensional nanostructured materials, Quantum Dots shell structures, metal oxides, semiconductors, composites, mechanical-physical-chemical properties.

- **SYNTHETIC ROUTES OF NANOMATERIALS** **(18 Hours)**

  Principle and relative merits of each technique for production of Nano-structures including ultra-thin films and multilayer by: (a) Laser Ablation technique, (b) Arc Discharge technique and (c) Mechanical Milling. Physico-chemical methods such as Chemical Vapor Deposition (CVD), Plasma, Sputtering, Hot-Wire Plasma Enhanced CVD method, and Self-assembly technique.

  Chemical methods: Synthesis of nanomaterials by precipitation and co-precipitation methods, Sol-Gel synthesis, Microemulsions synthesis, Hydrothermal and Solvothermal methods. Microwave assisted synthesis, Sonochemical assisted synthesis. Metal nanocrystals synthesis by polyol, and borohydrate reduction methods, Photochemical synthesis, Synthesis in supercritical fluids and Electrochemical synthesis, Synthesis of Core-Shell nanostructure, Organic –Inorganic Hybrids, Quantum dots (QDs), Carbon Nanotubes, Graphenenanosheets. Biological methods: Use of bacteria, and fungi. Role of plants in nanoparticle synthesis.

- **PROPERTIES, CHARACTERIZATION AND APPLICATIONS OF NANOMATERIALS** **(14 Hours)**

  Properties and size effect of nanomaterials, electrical, Mechanical, Magnetic, Optical and catalytic properties, Characterization methods, Applications of nanotechnology in sustainable development and technology.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. G. A. Ozin, A. C. Arsenault, L. Cademartiri, *Nanochemistry: A Chemical Approach to Nanomaterials*, 2nd Edition, The Royal Society of Chemistry, Cambridge, 2009.

2. C. N. R Rao, A. Muller, A. K Cheetham, *Nanomaterials Chemistry*, 1st Edition, Wiley-VCH, 2007.
3. G. Cao, *Nanostructures & Nanomaterials: Synthesis, Properties, and Applications*, 1st Edition, Imperial College Press, London, 2004.
4. M. Hosokawa, K. Nogi, M. Naito, Y. Yokoyama, *Nanoparticles Technology Handbook*, 1st Edition, Elsevier, 2007.
5. T. Pradeep, *NANO The Essentials: Understanding Nanoscience and Nanotechnology*, 1st Edition, Tata McGraw-Hill Publishing Company Ltd., New Delhi, 2007.

4. Additional Reading Material:

1. K. Klabunde, *Nano-chemistry*, 2nd Edition, Elsevier Publishers, 2013.

FOURTH YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - IV, SEMESTER - VIII

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Symmetry, Spectra & Magnetism	CY-402	3-1-4	06	100	25	60	40	225
2.	Chemistry of Natural Products	CY-404	3-1-4	06	100	25	60	40	225
3.	Physical Aspects of Molecular spectroscopy	CY-406	3-1-4	06	100	25	60	40	225
4.	Core Elective-2	CY-4YY	3-0-0	03	100	00	00	00	100
Total contact hours per week=27			**Total Credits=21**			**Total Marks=775**			

Elective-2 (CY-4YY)

Sr. No.	Code	Subject
1.	CY-422	Purification and Separation Methods in Chromatography
2.	CY-424	Fluorescence Spectroscopy
3.	CY-426	Polymer and Coating Technology
4.	CY-428	Organic Materials
5.	CY-432	Drugs and Dyes
6.	CY-434	Green Chemical Processing

SYMMETRY, SPECTRA & MAGNETISM

L	T	P	C
3	1	4	6

Scheme

CY402

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain principles and concepts of symmetry and group theory.
CO2	Justify the use of character tables and projection operator techniques.
CO3	Recognize the importance of symmetry and group theory in spectroscopy.
CO4	Illustrate inorganic electronic spectra.
CO5	Describe inorganic magnetism.

2. Syllabus:

- **SYMMETRY AND GROUP THEORY** **(20 Hours)**

  Group theory: The concept of group, Symmetry elements and symmetry operations, Assignment of point groups to inorganic molecules, Features of point groups and their character tables, Representations (matrices, matrix representations for C_2V and C_3V point groups irreducible representations), Character and character tables for C_2V and C_3V point groups. Symmetries of molecular orbitals in BF_3, C_2H_4 and B_2H_6. Applications of group theory to chemical bonding.

- **SPECTRA & MAGNETISM OF TRANSITION METAL COMPLEXES** **(22 Hours)**

  The energy terms, coupling schemes, spin-spin coupling, orbital coupling, spin-orbital coupling, R-S coupling, J-J coupling scheme, selection rules, relaxation of selection rules. Energy levels in an atom, Calculation of the number of the microstates Determining the Ground State, Term Symbols, Terms-Hunds Rule, Hole formulation (derivation of the Term Symbol for a closed sub-shell, derivation of the terms for a d2 configuration), Orgel diagrams and its application to electronic spectra of transition metal complexes, Charge transfer spectra, electronic absorption spectra of spin paired complexes, Jahn-Tellar effect and electronic spectra of complexes; properties of paramagnetic complexes, magnetic moment, antiferromagnetism and ferromagnetism.

(Total Lecture Hours: 42)

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3. Practicals:

1. Given a solution of $BaCl_2$ and $CaCl_2$ determine the amount of Ba gravimetrically and Ca volumetrically by oxalate method.
2. Estimation of Cu and Ni in the given solution containing $CuSO_4$ and $NiSO_4$.
3. To prepare the tetraamminecopper(II) sulphate monohydrate complex $[Cu(NH_3)_4\ (H_2O)]SO_4$ from copper sulphate ($CuSO_4.5H_2O$). To estimate the amount of Cu in the prepared sample volumetrically.
4. To estimate gravimetrically, the amount of lead present in the whole of the given solution of lead acetate (or lead nitrate) by precipitating it as lead chromate.
5. Determination of lanthanide by complexometric titrations.
6. Determination of actinides by complexometric titrations.
7. To prepare potassium trisoxalatochromate (III), $K_3[Cr(C_2O_4)_3]$.
8. To determine concentration of PO_4^{3-} ion spectrophotometrically.

4. Books Recommended:

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th Edition, Pearson Education India, 2006.
2. F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edition, Wiley, 2008.
3. B. Durrant, P. J. Durrant, *Introduction to Advanced Inorganic Chemistry*, 12th Edition, Longmans Green and Co., 1962.
4. H. H. Jaffe, M. Orchin, *Symmetry in Chemistry*, Dover Publications, 2003.
5. R. H. Crabtree, *The Organometallic Chemistry of Transition Metals*, 5th Edition, John Wiley and Sons, 2009.

5. Additional Reading Material:

1. J. D. Lee, *Concise Inorganic Chemistry*, 5th Edition, Blackwell Science, 1996.
2. C. J. Jones, *d - and f - block Chemistry*, 1st Edition, RSC, 2006.
3. R. S. Drago, *Physical Methods in Inorganic Chemistry*, 1st Edition, International Edn. East-West Press Pvt. Ltd., 1971.

CHEMISTRY OF NATURAL PRODUCTS

L	T	P	C
3	1	4	6

Scheme

CY404

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Identify and characterize various classes of natural products.
CO2	Review the biogenesis of various important natural products.
CO3	Acquire the skills to isolate and purify natural plant products.
CO4	Demonstrate the knowledge on the role of biomolecules and their importance.
CO5	Illustrate the properties, composition and biosynthesis of the natural products like terpenoids, steroids, phenylpropanoids and alkaloids.

2. Syllabus:

- **NATURAL PRODUCTS OF CHEMISTRY** **(25 Hours)**
  Primary and secondary metabolites, general methods for isolation and structural determination of natural products,
  Terpenoids: Classification, occurrence, isoprene rule, structure determination, stereochemistry, biosynthesis and synthesis of citral, geraniol, α-terpeneol, menthol. Vitamins A, D and E.
  Steroids: Classification, occurrence, basic skeleton, Diel's hydrocarbon and stereochemistry, synthesis of cholestrol, progestrone and testosterone.
  Alkaloids: Structure determination, stereochemistry, biosynthesis and synthesis of nicotine, quinine and morphine.

- **NATURAL PIGMENTS** **(05 Hours)**
  Classification of natural pigments, structure determination of porphine, porphyrin, Hb, Chl, flavones, and flavonoids.

- **AMINO ACIDS, PEPTIDES AND PROTEINS** **(06 Hours)**
  Classification, acid-base behaviour, Isoelectric point and electrophoresis. Structure and confirmation of peptides and proteins, Determination of structure of peptide, classical peptide synthesis solid phase peptide synthesis, Structure of peptide and proteins, Classification and function of proteins, denaturation of proteins.

- **BIO-ORGANIC CHEMISTRY** **(06 Hours)**
  Organic reactions in laboratory and in biological systems. Nature of biomolecular interactions. Stereo-specificity and rate enhancement in enzyme catalysed reactions. Mechanism of hydrolysis of esters, amides, phosphoesters in biological systems; C-C and C=C bond formation, oxidation, reduction and decarboxylation. Remote functionalisation cyclisation reactions. Hydrophobicity and organized assemblies.

(Total Lecture Hours: 42)

3. Practicals:

1. Separation of aminoacids by paper and thin layer chromatography.
2. Isolation of Embellin from Embeliaribes.
3. Isolation of peperanol from piperine.
4. Isolation of nicotine from tobacco.
5. Isolation of Eucalyptus oil from Eucalyptus leaves.
6. Isolation of Curcumin from Turmeric powder.
7. Estimation of phenol, acetone and aniline.
8. Soxhlet extraction of caffeine from tea leaves.
9. Separation of *ortho* and *para*nitroanilines by column chromatography.

4. Books Recommended:

1. I. L. Finar, *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*, Volume 1 & 2, 5th Edition, Person Education India, 2002.
2. M. Cox, D. L. Nelson, *Lehninger Principles of Biochemistry*, 6th Edition, W. H. Freeman and Company, 2013
3. H. Dugas, *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*, 3rd Edition, Springer-Verlag, 2005.
4. D. E. Metzler, *Biochemistry - The Chemical Reactions of a Living Cell*, 2nd Edition, Academic Press, 2003.
5. K. Nakanishi, T. Goto, S. Ito, S. Natori, S. Nozoe, *Natural Products Chemistry*, Volume 3, 1st Edition, University Science Books, USA, 1991.

5. Additional Reading Material:

1. D. H. R. Barton, K. Nakanishi, O. Meth-Cohn, *Comprehensive Natural Products Chemistry*, Volume 1-9, 1st Edition, Pergamon, 2001.
2. H. Dugas, *Bioorganic Chemistry Frontiers*, Volume 2, Page1-252, Springer-Verlag, 1991.
3. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, A. R. Tatchell, *Vogel's Textbook of Practical Organic Chemistry*, 5th Edition, Pearson India, 2005.
4. R. K. Bansal, *Laboratory Manual of Organic Chemistry*, 5th revised Edition, New Age International Pvt. Ltd. Publishers, 2008.

PHYSICAL ASPECTS OF MOLECULAR SPECTROSCOPY

L	T	P	C
3	1	4	6

CY406

Scheme

1. Course Outcomes (Cos):

At the end of the course students will be able to:

CO1	Gain fundamental knowledge of symmetry and symmetry operations.
CO2	Employ concepts of molecular spectroscopy and selection rules.
CO3	Explain the structural elucidation by molecular spectroscopy.
CO4	Demonstrate structural characterization of a molecule through spectroscopy.
CO5	Perform the experiments related to physical chemistry approach which includes Kinetics, Conductometry, Colorimetry, pH-metry, Potentiometry and titration.

2. Syllabus:

- **MOLECULAR SYMMETRY** **(12 Hours)**
  Symmetry elements and operations, Group postulates, Point Groups, Great Orthogonality Theorem (G.O.T.), Character Table for point groups, Crystallographic symmetry. Standard reduction formula, Normal Modes of Vibration of H_2O, NH_3 and BF_3 molecules.

- **MOLECULAR SPECTROSCOPY- I** **(15 Hours)**
  Spectroscopy - Nature of electromagnetic radiation, range of wavelength, Transition moment integral (qualitative idea) and allowed transitions, Separation of electronic and nuclear motion, Born-Oppenheimer approximation, Signal to noise ratio, Width and intensity of transition, line broadening Rotational spectroscopy, Rigid rotor (diatomic only), Selection rule, Spectrum: position and intensity of spectral lines. Non-rigid rotor and its effect on energy levels, Selection rule and spectrum, Applications, Isotope effect.

- **MOLECULAR SPECTROSCOPY – II** **(15 Hours)**
  Electromagnetic radiation with wavelength and energy. Molar refraction, polarizability, dipole moment, molecular structure and dipole moment, Radio frequency, Microwave, IR, UV/ visible region, pure rotational spectra, Vibrational and Vibrational-Rotational spectra, Raman spectra. Calculation of bond-length. Vibrational rotational spectra, Hooke's law, vibrational energy level. Anharmonic Vibration. Numericals.

(Total Lecture Hours: 42)

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3. Practicals:

1. To study the triangular phase diagram (solubility curve) for a ternary system of liquids: Acetic acid + Chloroform + water.
2. To study the effect of substituents of dissociation constant of benzoic acid (weak acid) by conductance method.
3. To determine the composition of the complex formed by the reaction between Zn (II) with $K_4Fe(CN)_6$ potentiometrically.
4. Determination of complex formation between Cu^{2+} and NH_3 by distribution method.

5. To determine the rate constant of saponification of ethyl acetate at two different temperatures and calculate the energy of activation of the reaction.
6. To determine the CMC of a surfactant (SDS) at three different temperatures in aqueous solution by conductance method & calculate Gibb's energy for micellization.
7. To determine the amount of Fe^{2+} by adding EDTA using spectrophotometrically.
8. Determination of radius of a molecule (glycerol) by Viscosity method.

4. Books Recommended:

1. J. M. Hollas, *Modern Spectroscopy*, 4th Edition, Wiley, 2004.
2. C. N. Banwell, Elaine M. Mc Cash, *Fundamentals for Molecular Spectroscopy,* 4th Edition, McGraw-Hill, 1994.
3. N. Levine, *Quantum Chemistry*, 4th Edition, Prentice Hall, Englewood Cliffs, New Jersey, 1991.
4. G. M. Barrow, *Physical Chemistry*, 6th Edition, McGraw-Hill, Kogakusha Ltd., New Delhi, 1973.
5. S. Maity, N. Ghosh, *Physical Chemistry Practical*, 1st Edition, New Central Book Agency (P) Ltd., India, 2012.

PURIFICATION AND SEPARATION METHODS IN CHROMATOGRAPHY

CY422

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (Cos):

At the end of the course students will be able to:

CO1	Interpret the role of analytical techniques in separation and identification of various chemical species.
CO2	Acquire a deep knowledge on chromatography.
CO3	Apply the basics of the separation and chromatographic techniques in multidisciplinary areas.
CO4	Develop the skill to apply the advances in chromatography in separation.
CO5	Propose the importance of purity of product in industrial use.

2. Syllabus:

- **SEPARATION TECHNIQUES** **(09 Hours)**

  Distribution law, thermodynamic derivation, application, process of extraction, factors affecting extraction, techniques for solvent extraction, conventional, liquid membranes, bulk, supported and emulsified, solid phase extraction (SPE), ion-exchange, conventional membranes. quantitative treatment of solvent extraction equilibria, classification of solvent extraction system, types of extraction system, advantages of solvent extraction system, applications of liquid extraction, solvent extraction methods in metallurgy, solid liquid extraction.

- **CHROMATOGRAPHY** **(08 Hours)**

  Principle, methods of elution, ideal and non-ideal chromatography, plate theory, rate theory, reasons for broadening of lands, Van-Deemter equation and significance of terms involved, optimum velocity, resolution, methods to improve resolution. introduction to chromatographic techniques: paper chromatography, Thin Layer Chromatography (TLC) and Column Chromatography.

- **GAS CHROMATOGRAPHY (GC)** **(09 Hours)**

  Principle, different types of GC, mobile phase and criteria for its selection, stationary phase, sample introduction system, columns, Stationary phases used in GSC and GLC, difference between GSC and GLC, supports for liquid stationary phases, Selection of columns, packed, WCOT, SCOT, FSOT, Detectors: FID, TCD, FPB, ECD, TID - merits and demerits, temperature programming in GC, derivatisation in GC, Qualitative analysis from retention parameters, Quantitative analysis.
  GC-Mass Spectroscopy Waston-Biemann Separator, Ryhage Separator, Llewellyn Separator, Instrumentation, Applications.

- **LIQUID CHROMATOGRAPHY** **(09 Hours)**

  Principle of LC, instrument and significance of each component, Pumps, Guard column, Stationary phases (solid, liquid), Mobile Phases, Bonded phase supports, Detectors - Fluorescence detector, RI detector, electrochemical detector, Normal phase and Reversed phase. Introduction to HPLC and UPLC.
  LC Mass Spectroscopy
  LC/MS interfaces, solvent removal and ionization, atmospheric-pressure interfaces, electro spray Interface, ion spray interface, secondary detectors.

- **ION-EXCHANGE CHROMATOGRAPHY** **(07 Hours)**
  Introduction: principle of exchange, resins used swelling, capacity of resin and its determination, effect of different parameters on exchange behavior, techniques of IEC, eluent suppressor column. Applications.

(Total Lecture Hours: 42)

3.Books Recommended:

1. D. Harvey, *Modern Analytical Chemistry*, 3rd Edition, McGraw Hill Publication, New York, 2000.
2. R. M. Verma, *Analytical Chemistry – Theory and Practice*, 3rd Edition, CBS Publication, New Delhi, 2004.
3. J. M. Miller, *Chromatography Concepts and Contrasts*, 2nd Edition, Wiley-Interscience, 2001.
4. D. A. Skoog, F. J. Holler, T. A. Nieman, *Principles of Instrumental Analysis*, 6th Edition, 2006.
5. R. L. Grobe, *Modern Practice of Gas Chromatography*, 4th Edition John Wiley Interscience, 2004.

FLUORESCENCE SPECTROSCOPY

L	T	P	C
3	0	0	3

Scheme

CY424

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain basics of fluorescence spectroscopy.
CO2	Explore the applications of fluorescence spectroscopy.
CO3	Acquire knowledge on fluorescent sensing mechanisms.
CO4	Identify in-vivo use of fluorescence microscopy.
CO5	Describe various advanced techniques of fluorescence spectroscopy.

2. Syllabus

- **INTRODUCTION TO FLUORESCENCE SPECTROSCOPY** **(12 Hours)**
  Introduction: Jabloski diagram, Stokes shift, delayed fluorescence, emission and excitation spectra, quantum yield; solvents and environmental effects; Instrumentation, fluorophores: intrinsic and extrinsic fluorophores, red and NIR fluorophores, fluorescent organic and inorganic nanoparticles, lanthanides and metal complexes as fluorophore, Fluorescent Proteins, Miscellaneous Probes; time-domain lifetime measurements.

- **FLUORESCENCE QUENCHING** **(08 Hours)**
  Quenching of fluorescence, collision quenching, static and dynamic quenching, Stern-Volmer equation, intramolecular quenching, Quenching and Membrane Systems, application of quenching to proteins.

- **ENERGY TRANSFER** **(08 Hours)**
  Characteristics of resonance energy transfer (RET), theory of energy transfer, Determination of distances using RET, RET in ensembles of donors and acceptors, RET in three dimensions, Effect of viscosity, Effects of dimensionality on RET, Effects of restricted geometries on RET, RET between like molecules. Excitation energy migration in assemblies of chromophores, RET within a pair of like chromophores, RET in assemblies of like chromophores, Weber's red-edge effect, RET sensors, Biochemical and other applications.

- **POLARIZATION AND ANISOTROPY** **(08 Hours)**
  Polarized Light and Photoselection of Absorbing Molecules, Characterization of the Polarization State of Fluorescence, Instantaneous and Steady-State Anisotropy, Additivity Law of Anisotropy, Relation between Emission Anisotropy and Angular Distribution of the Emission Transition Moments, Case of Motionless Molecules with Random Orientation, Effect of Rotational Motion, Applications.

- **FLUORESCENT SENSING** **(06 Hours)**
  Introduction: design and applications of fluorescence sensing, Mechanism of sensing: sensing by collision quenching, Energy-transfer sensing, aggregation-induced emission based sensing, PET probes, excimer-monomer based probes, probes with other sensing mechanisms, sensing with fluorescent nanomaterials, biosensors, Molecular Beacons, Introduction of Fluorophores into Living Cells, Bioimaging.

(Total Lecture Hours: 42)

3. Books Recommended:

1. J. R. Lakowicz, *Principle of Fluorescence Spectroscopy*, 3rd Edition, Springer, 2006.
2. B. Valeur, *Molecular Fluorescence: Principles and Applications*, 2nd Edition, Wiley, 2012.
3. D. M. Jameson, *Introduction to Fluorescence*, 1st Edition, CRC Press, 2014.
4. J. R. Albani, *Principles and Applications of Fluorescence Spectroscopy*, 1st Edition, Wiley-Blackwell, 2007.
5. A. Sharma, S. G. Schulman, *Introduction to Fluorescence Spectroscopy*, 1st Edition, Wiley, 1999.

POLYMER AND COATING TECHNOLOGY

L	T	P	C
3	0	0	3

Scheme

MC426

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Provide a broad and fundamental knowledge of the synthetic polymers.
CO2	Emphasis on the processing techniques, along with the production of polymers.
CO3	Identify general and up-to-date information on raw materials, coating formulation, properties, and application.
CO4	Gain knowledge about the emerging technologies in polymers and coatings, and convey the latest developments demonstrating practical aspects and utility of recent developments and discoveries.
CO5	Explain about ingredients and composition of industrial, automotive, aerospace, wood finishes, road marking paint, novelty finishes and powder coatings.

2. Syllabus:

- **INTRODUCTION** **(08 Hours)**
  History of surface coating, current situation in coating technology, future forecast, economic importance of coatings, classification and structure of coatings.

- **COATING SYSTEM** **(12 Hours)**
  Raw Materials for coatings: film formers, solvents, pigments and fillers, additives, composition of coating materials, substrates, pre-treatment, coating process.

- **ANTICORROSIVE COATING** **(06 Hours)**
  Anticorrosive pigments, inhibitive pigments, sacrificial pigments, barrier pigments, organic inhibitors, sol-gel and hybrid coating, polymeric anticorrosive coatings.

- **POWDER COATING** **(06 Hours)**
  Resins used in powder coatings, additives, powder production and application.

- **SPECIAL PURPOSE COATING** **(10 Hours)**
  Automotive coatings, marine coatings, aerospace and aircraft coatings, self-cleaning and self-healing coatings.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. T. Brock, M. Groteklaes, P. Mischke, *European Coatings Handbook*, 2nd Revised Edition, Vincentz, 2010.
2. G. Gunduz, Chemistry, *Materials and Properties of Surface Coatings: Traditional and Evolving Technologies*, Destech Publications, Inc., 2016
3. P. Deligny, N. Tuck, *Resin for Surface Coatings*, Volume 1, 2 and 3, 2nd Edition, John Wiley and Sons, 2001.

4. T. J. Miranda, *Surface Coatings: Raw Materials and Their Usage*, Volume 1, 3rd Edition, Springer, 1993.
5. Z. W. Wicks, Jr., F. N. Jones, S. P. Pappas, D. A. Wicks, *Organic Coatings: Science and Technology*, Wiley Interscience, 2007.

4. Additional Reading Material:

1. NIIR Board, *Modern Technology of Paints, Varnishes and Lacquers*, 2nd Edition, Asia Pacific Business Press Inc., 2007.
2. P. Oldring, P. Lam, *Waterborne and Solvent Based Surface Coatings Resins and Their Applications: Acrylics*, Volume 1, 1st Edition, SITA Technology, 1996.

ORGANIC MATERIALS

CY428

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Impart knowledge in fundamental aspects of organic materials.
CO2	Acquire knowledge on the preparation and properties of organic materials.
CO3	Gain knowledge on the synthetic strategies for preparation of multifunctional organic materials.
CO4	Recognize the basic knowledge on the role of organic materials in drug delivery.
CO5	Have an appreciation on the unique properties of organic materials and their applications.

2. Syllabus:

- **ORGANIC MATERIALS** **(16 Hours)**
  Introduction, definition, structure, types of organic materials, general method of preparation, properties, detection, and characterization of organic nanoparticles: hydrophobic drugs, protein, peptide, lipid, cyclodextrin, polysaccharides. Nanocochleates, prospects and future challenges.carbon molecules – nature of the carbon bond – new carbon nanostructures; carbon nanoclusters. molecular self-assemblies, surface engineering. Preparation of bionanomaterials, nanoparticles and microorganisms, microbial synthesis of nanomaterials, biological methods for synthesis of nano-emulsions using bacteria, fungi and actinomycetes, plants based nanoparticle synthesis, nanocomposite biomaterials – fibres, devices and structures, nanobio-systems.

- **SMART MATERIALS** **(06Hours)**
  Synthesis of smart materials, types of smart materials, micro sensors, hybrid smart materials, electro-Rheological (fluids) smart materials, and piezoelectric smart materials.

- **FUNCTIONAL ORGANIC MATERIALS** **(08Hours)**
  3-D-carborich pi-systems - nanotubes and segments; strategic advances in chromophore and materials syntheses; self-assembly strategies towards multifunctional materials; molecular muscles, switches and electronics; electronic interaction and structure.

- **NANOTECHNOLOGY IN DRUG DELIVERY** **(12Hours)**
  Nanoparticle in drug delivery, controlled release, organic materials future application understanding for treatment. Nanopowder and nanocrystals, targeting ligands applications of nanoparticle in drug delivery, cancer treatment, mediated delivery of sirna, nanonephrology, nanosystems in inflammation, targeting macrophages to control inflammation, tissue regeneration, growth and repair, tissue bioengineering; future understanding for treatment, drug delivery technology significance, impact of drug discovery and development. Applications of nanobiotechnology: organic materials cytotoxicity, green organic particle production; biocompatbility; Applications of green nanotechnology; use of organic materials impact on nanotechnologies, biodiversity, resource conservation, ecosystems.

(Total Lecture Hours: 42)

3. Books Recommended:

1. M. Schwartz, *Smart Materials*, CRC Press, 1st Edition, 2008.
2. S. V. Bhat, *Biomaterials*,Springer Netherlands, 1st Edition 2002.
3. G. L. Hornyak, J. Dutta, H. F. Tibbals, A. K. Rao, *Introduction to Nanoscience*, CRC Press, 1st Edition, 2008.
4. G. A. Ozin, A.C. Arsenault, L. Cademartiri, *Nanochemistry: A Chemical Approach to Nanomaterials*, The Royal Society of Chemistry, Cambridge, 2nd Edition, 2009.
5. G. Cao, *Nanostructures & Nanomaterials: Synthesis, Properties, and Applications*, Imperial College Press, London, 2004.

4. Additional Reading Material:

1. T. Vo-Dinh, *Nanotechnology in Biology and Medicine: Methods, Devices and Application*, CRC Press, 2007.
2. A. M. Hillery, *Drug Delivery and Targeting*, CRC Press, 2002.
3. J. J. T. Müller, U. H. F. Bunz (Eds), *Functional Organic Materials: Syntheses, Strategies and Applications*, Wiley-VCH, 2007.

DRUGS AND DYES

CY432

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Acquire deep knowledge of theories of colour and chemical constitution.
CO2	Describe various dyestuff and categorize their applications.
CO3	Explain procedures followed in drug design and various theories of drug activity.
CO4	Interpret pharmacokinetics and pharmacodynamics.
CO5	Describe the concept of the therapeutic concentration range.

2. Syllabus:

- **THEORY OF COLOUR AND CHEMICAL CONSTITUTION** **(06 Hours)**
  Auxochrome, chromogen, chromophore of colour chemistry, colour and chemical constitutions. Theories to explain relation between colour and chemical constitutions: Witt's theory, Armstrong theory, Baeyer's theory, Nietzki's theory, Watson's theory. Modern theories: Valence bond theory (resonance theory) and Molecular orbital theory.

- **SYNTHESIS OF DYESTUFF AND PIGMENT OF VARIOUS CLASSES** **(05 Hours)**
  Chemical Synthesis of Nitro and Nitroso dyes; Azo dyes such as Direct, Acid, Basic, Mordant, Disperse dye. Diphenyl methane dyes (DPM); Triphenyl Methane Dyes (TPM); Phthalocyanine; Xanthene dyes; Heterocyclic dyes such as acridine dyes; Indigo and Thioindigo; Solubilised vat dyes; Anthraquinon dyes such as Mordant vat, disperse and acid dyes; Reactive dyes such as procion dyes and vinyl sulphone dyes.

- **NON-TEXTILE APPLICATION OF DYES** **(03 Hours)**
  Food colours, cosmetic dyes, dyes for paper and printing inks, dyes for paints, High tech dyes.

- **FLUORESCENT BRIGHTENING AGENTS** **(04 Hours)**
  General account, classification of FBA base on chemical constitution with examples, Stilbene and Coumarin derivatives of FBA, synthesis of Tinopal BV, Blankophor -B, Blankophor-G , 3-phenyl-7 methoxy coumarin, 4 methyl –3 phenyl-7-aminocoumarin.

- **DRUG DESIGN** **(06 Hours)**
  Procedure followed in drug design, Concept of prodrugs and soft drugs, Theories of drug activity: Occupation theory, rate theory, induced fit theory. Concepts of drug receptors, Elementary treatment of drug receptor interactions, LD-50, ED-50.

- **PHARMACOKINETICS** **(06 Hours)**
  Introduction of drug absorption, disposition, elimination using pharmacokinetics, important pharmacokinetics parameters in drug disposition and in therapeutics, Importance of pharmacokinetics in drug design.

- **PHARMACODYNAMICS** **(06 Hours)**
  Introduction, elementary treatment of enzyme stimulation, enzyme inhibition, drug metabolism, phase-I, Phase-II reactions, biotransformation.

- **SYNTHESIS OF SELECTIVE DRUGS** **(06 Hours)**
  Ciprofloxacin, Ibuprofen, Atenolol, Captopril, Diazepam, Chloroquine, Barbiturates, Miconazole, Biotin, Ethambutol, Ranitidine, and Omeprazole.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. R. Christie, *Colour Chemistry*, 2nd Edition, Royal Society of Chemistry, 2015.
2. G. R. Chatwal, *The Synthetic Dyes*, 4th Edition, Himalaya Publishing House, 2016.
3. M. Sitting, *Pharmaceutical Manufacturing Encyclopaedia*, 3rd Edition, William Andrew Publishing, 2006.
4. S. D. Seth, V. Seth, *Textbook of pharmacology*, 3rd Edition, Elsevier 2009.
5. A. Korolkovas, *Essentials of Medicinal Chemistry*, John Wiley & sons, 2nd Edition, 2008.

GREEN CHEMICAL PROCESSING

L	T	P	C
3	0	0	3

CY434

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain green chemistry concepts and its significance for environment sustainability.
CO2	Differentiate between conventional and green raw materials.
CO3	Design green process and analyze sustainability of materials.
CO4	Analyze sustainability of chemical processes.
CO5	Establish application of green chemistry in multidisciplinary areas including pharmaceutical, petrochemical, storage and green fuel production.

2. Syllabus:

- **ENVIRONMENT SUSTAINABILITY OF CHEMICAL PROCESSES** **(05 Hours)**
  Introduction to green chemistry, criteria for selection of green technologies, renewable feedstock, sustainable solvents and auxiliaries,waste minimization and design for degradation.

- **GREEN SYNTHETIC ROUTES** **(10 Hours)**
  Chemie Douce approach of material synthesis, Intercalation, Anchoring, Pillaring, Sonochemical method, Microwave synthesis, Mechanochemical synthesis, Electrochemical synthesis and Photochemical synthesis.

- **GREEN MATERIALS** **(10 Hours)**
  Zeolites, hydrocalcites, heteropoly acids, metal organic frameworks, sulfated zirconia and ionic liquids as catalysts.

- **APPLICATIONS OF GREEN PROCESSES** **(17 Hours)**
  (i) For active pharma ingredients (API)
  (ii) For polymers
  (iii) For green fuel production and polymer membrane fuel cells
  (iv) For CO_2 utilization and carbon credit
  (v) For biomass to value added products

(Total Lecture Hours: 42)

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3. Books Recommended:

1. M. Lancaster, *Green Chemistry: An Introductory Text*, 1st Edition, RSC, 2002.
2. E. Lichtfouse, J. Schwarzbauer, *Green Materials for Energy, Products and Depollution (Environmental Chemistry for a Sustainable World)*, 1st Edition, Springer, 2013.
3. P. Wasserscheid, A. Stark, *Handbook of Green Chemistry*, Volume 6, Ionic liquids, 1st Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2013.
4. G. Rothenberg, *Catalysis: Concepts and Green Applications*, 2nd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2008.
5. V. K. Ahluwalia, *Green Chemistry: Environmentally Benign Reactions*, 2nd Edition, Ane Books Pvt. Ltd, 2009.

4. Additional Materials

1. P. T. Anastas, J. C. Warner, J. Warner, *Green Chemistry: Theory and Practice*, 1st Edition, Oxford University Press, 2000.
2. R. XU, W. Pang, O. Huo, *Modern Inorganic Synthetic Chemistry*, 2nd Edition, Elsevier, 2010.

FIFTH YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - V, SEMESTER – IX

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Seminar	CY-501	0-0-2	01	00	00	20	30	50
2.	Dissertation Preliminaries	CY-503	0-0-16	08	00	00	80	120	200
3.	Industrial Visit(s)	CY-505	0-0-0	01	00	00	20	30	50
4.	Elective-3	CY-5XX	3-0-0	03	100	00	00	00	100
	Elective-4	CY-5YY	3-0-0	03	100	00	00	00	100
Total contact hours per week=24			Total Credits=16			Total Marks=500			

Elective-3 (CY-5XX)

Sr. No.	Code	Subject
1.	CY-521	Synthetic Dyes for Textile Processing
2.	CY-523	Green Solvents
3.	CY-525	Catalysis
4.	CY-527	Spectroscopic Techniques in Inorganic Chemistry

Elective-4 (CY-5YY)

Sr. No.	Code	Subject
1.	CY-529	Heterocycles and Organic Synthesis
2.	CY-531	C-H Functionalization
3.	CY-533	Supramolecular Chemistry
4.	CY-535	Physical Methods of Structure Determination

FIFTH YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - V, SEMESTER – X

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Dissertation	CY-502	0-0-24	12	00	00	160	240	400
Total contact hours per week=24			**Total Credits=12**		**Total Marks=400**				

SYNTHETIC DYES FOR TEXTILE PROCESSING

L	T	P	C
3	0	0	3

CY521

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explain the chemistry of colouring matters, its origin, types and importance.
CO2	Provide basic principle and chemistry of various dyes with their properties.
CO3	Identify the fundamentals aspects of colour, relation between colour and chemical constitution of dyes.
CO4	Explore the use of synthetic dyes to develop and familiarize with basic dyeing techniques.
CO5	Provide technical knowhow for coloration and printing of different textiles.

2. Syllabus:

- **TEXTILE DYEING** **(08 Hours)**
  Introduction, Dyeing Technology, Principles of Dyeing, bath Dyeing Technology, Continuous and Semi Continuous Dyeing, printing, Dispensing Dyes and Chemicals, Standardization of Textile Dyes, Laboratory Dyeing Techniques.

- **REACTIVE DYES AND DIRECT DYES ON CELLULOSE FIBERS** **(06 Hours)**
  Reactive dyes: Introduction, Chemistry, synthesis, Dyeing Techniques for Cellulose, Reactive Dyes on Wool, Silk and Polyamide Fibers, Reactive Dyes for Printing on Cellulose.
  Direct Dyes: Dyeing Principle, Dyeing Parameters, Dyeing Techniques, After treatment, Direct Dyes for Fiber Blends.

- **ANTHRAQUINONE VAT DYES ON CELLULOSIC FIBERS** **(04 Hours)**
  Introduction, Chemistry and synthesis of anthraquinone vat dyes, Principles of Vat Dyeing, The Vat Dyeing Process, Vatting, Dye Absorption in the Exhaustion Process, Oxidation, After treatment (Soaping), Dyeing Techniques, Vat Dyes for Fiber Blends, leuco Esters of Vat Dyes on Cellulosic Fibers.

- **DYEING WITH INDIGO AND SULFUR DYE** **(06 Hours)**
  Indigo dye: Introduction, Chemistry, synthesis, Dyeing Technique on Cotton, Indigo on Wool, : Sulphur dye: Introduction, Chemistry, synthesis, Sulfur Dyes on Cellulosic Fibers: Types and Mode of Reaction, Additives to the Dye Bath, The Dyeing Process, Dyeing Techniques, Combination with Other Dyes.

- **AZO DYES ON CELLULOSIC FIBERS** **(06 Hours)**
  Introduction, Chemistry, synthesis, Application of Azo Dyes, Dyeing Processes on Cellulosic Fibers, Printing with Azo Dyes on Cellulosic Fibers.

- **DISPERSE DYES ON POLYESTER AND OTHER MAN-MADE FIBERS** **(06 Hours)**
  Introduction, Chemistry, synthesis, General Aspects, dyeing in Aqueous Liquor, Thermosol Process, Dyeing Processes for Polyester Fibers with Disperse Dyes, Suitability of Disperse Dyes for Different Applications, Dyeing from Aqueous Dye Baths, special Dyeing Processes, Continuous and Semicontinuous Dyeing Processes, Dyeing of PES Microfibers, Dyeing of Modified PES

Fibers, Printing with Disperse Dyes on Man-Made Fibers, After treatment, dyeing Blends Containing Polyester Fibers, Polyester Cellulose Blends, Polyester Wool Blends.

- **FASTNESS OF COLOURED TEXTILES** **(06 Hours)**
  Colour and light fastness, fastness test and properties, fastness test towards processing conditions and condition in use.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. R. M. Christie, *Colour Chemistry*, 2nd Edition, The Royal Society of Chemistry, 2015.
2. K. Hunger, *Industrial Dyes: Chemistry, Properties, Applications*, 3rd Revised Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim. 2003.
3. V. A. Shenai, *Chemistry of Dyes and Principles of Dyeing*, Sevak Publications, 1983.
4. H. A. Lubs, *The Chemistry of Synthetic Dyes and Pigments*, 4th Edition, Krieger Publishing Company, 1977.
5. K. Venkatraman, *Chemistry of Synthetic Dyes*, Volume 1-5, 1st Edition, Academic Press, New York and London, 1972.

4. Additional Reading Materials:

1. K. M. Shah, *"Handbook of Synthetic Dyes and Pigments"*, Volume 1-2, 2nd Edition, Multi-tech Publishing Co., 1998.
2. G. R. Chatwal, *Synthetic Dyes*, 3rd Edition, Himalaya Publishing House, 2007.

GREEN SOLVENTS

CY523

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Gain knowledge in fundamental aspects of Green Chemistry.
CO2	Acquire knowledge on the preparation and properties of Green Solvents.
CO3	Develop the synthetic strategies for the preparation of tailor made Ionic Liquids, Deep Eutectic Solvents and Supercritical Fluids.
CO4	Demonstrate the basic knowledge on the role of Green Solvents in diverse applications.
CO5	Have a knowledge on the unique properties of Green Solvents and their industrial applications.

2. Syllabus:

- **GREEN CHEMISTRY PRINCIPLES** **(06 Hours)**
  Principles of green chemistry, Green pathways for chemical syntheses, designing safer and energy efficient solvents, real time analysis for pollution prevention, and inherently safer chemistry for accident prevention.

- **IONIC LIQUIDS** **(14 Hours)**
  Introduction, Synthesis and Purification of Ionic Liquids (ILs), Physicochemical properties of ILs, ILs as Catalysts, Bio-ILs, ILs in synthesis, Green Synthesis of ILs for Green Chemistry, Thermodynamic Properties of liquid mixtures containing ILs, Surface Active ILs, ILs in Drugs, Biotransformations in ILs, Challenges to the Commercial production of ionic liquids.

- **DEEP EUTACTIC SOLVENTS** **(14 Hours)**
  Introduction – Composition of Deep Eutectic Solvents (DES), Physicochemical Properties of DESs, natural DESs, Applications of DES in Removal of Surface Contaminants, DES as Unconventional Media for Multicomponent Reactions, Applications of DESs in Metal Processing, Bio-transformations in DESs.

- **SUPERCRITICAL FLUIDS** **(08 Hours)**
  Introduction, Properties of Supercritical Fluids, Supercritical Fluids as Media for Chemical Reactions, Phase Equilibria in Near-Critical Solutions, Solvation in Supercritical Fluids, Homogeneous Organic Reactions as Mechanistic Probes in Supercritical Fluids, Supercritical Fluids in Heterogeneous Catalysis, Super critical Fluids in nanotechnology, Supercritical Carbon Dioxide and its applications.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. P. Wasserscheid. T. Welton, *Ionic Liquids in Synthesis*, 2nd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, 2008.
2. R. D. Rogers, K. R. Seddon, *Ionic Liquids as Green Solvents: Progress and Prospects*, American Chemical Society: Washington, DC (Distributed by Oxford University Press), 2003.

3. M. Yizhak, *Deep Eutectic Solvents*, 1st Edition, Springer International Publishing, Springer Nature Switzerland AG, 2019.
4. P. G. Jessop, W. Leitner, *Chemical Synthesis Using Supercritical Fluids*, 2nd Edition, Wiley-VCH Verlag GmbH VCH, Weinheim, 1999
5. E. Kiran, P. G. Debenedetti, C. J. Peters, *Supercritical Fluids: Fundamentals, and Applications*, 2nd Edition, Springer Netherlands, Springer Science, Business Media Dordrecht, 2000.

4. Additional Reading Material:

1. M. F. Kemmere, T. Meyer, *Supercritical Carbon Dioxide: In Polymer Reaction Engineering* (Green Chemistry), Wiley-VCH, 2005.
2. J. R. Williams, A. A. Clifford, *Supercritical Fluid Methods and Protocols*, Springer, Humana Press, 2000.

CATALYSIS

CY525

L	T	P	C
3	0	0	3

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Summarize basics and principle of catalysis and their potential use to produce environmental and industrial catalysts.
CO2	Apply fundamentals of catalyst preparation, develop characterization skills and evaluate catalyst
CO3	Interpret surface characterization data of catalysts, correlate structure and properties of catalysts and how this insight can be used to design new catalysts.
CO4	Discuss various spectroscopic and thermal techniques can be used to characterize catalytic materials.
CO5	Compile and propose new applications of catalysis in multidisciplinary areas including pharmaceutical, petrochemical, alternative energy, biorefineries etc.

2. Syllabus:

- **INTRODUCTION TO CATALYSIS CONCEPTS AND CLASSIFICATION (06 Hours)**
  Activation energy, activity, selectivity, stability, enantioselectivity, promoter, concept of TON and TOF, catalyst deactivation, life cycle of catalysts, Introduction to homogeneous catalysis, heterogeneous catalysis, homogenized heterogeneous catalysis, environmental catalysis, phase transfer catalysis, biocatalysis, photocatalysis, etc.

- **CATALYST TYPES (07 Hours)**
  Metal based catalysts, metal oxides, metal nanoparticles, supported catalysts, solid acid catalysts, shape selective catalysts.

- **CATALYSTS PREPARATION METHODS (10 Hours)**
  Precipitation, Impregnation, Sol-gel method, dry-gel method, template method, hydrothermal method, vapour phase method, microwave method, solid state crystallization method, ion exchange and catalyst preparation by functionalization and an overview of commercial manufacturing of catalysts.

- **METHODS FOR CATALYST CHARACTERIZATION (12 Hours)**
  Catalyst characterization by thermal methods, Surface area characterization by BET method, acidity and basicity measurements by NH_3-TPD method and CO_2 adsorption method, catalyst characterization by spectral (X-Ray, IR, NMR) and electron microscopic methods (SEM and TEM).

- **ENVIRONMENTAL AND INDUSTRIAL APPLICATIONS OF HETEROGENOUS CATALYSIS (07 Hours)**
  Applications of catalysis inorganic transformations, petrochemical and fertilizer industries, bio-energy production from biomass, etc.

(Total Lecture Hours: 42)

3. Books Recommended:

1. G. C. Bond, *Catalysis by Metals*, 2nd Edition, Academic Press: London, 1962.
2. J. W. Niemantsverdriet; *Spectroscopy in Catalysis*, 3rd Edition, Wiley-VCH Publications, Netherlands, 2007.
3. J. Cejka, A. Corma, S. Zones, *Zeolites and Catalysis Synthesis, Reactions and Applications*, 1st Edition, Wiley-VCH Verlag GmbH & Co. KGaA, 2009.
4. N.M. Gupta, V. B. Kartha, R. A. Rajadhyakha, *Spectroscopic Methods in Heterogeneous Catalysis*, TATA McGraw Hill, 1989.
5. G. Rothenberg, *Catalysis: Concepts and Green Applications*, 2nd Edition, Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim, 2008.

4. Additional Reading Material:

1. C. N. R. Rao and K. Biswas, *Essentials of Inorganic Materials Synthesis*, Wiley –Blackwell, 1st Edition, 2015.
2. B. Pottathara, S. Thomas, V. Kokol, *Nanomaterials Synthesis, Design, Fabrication and Applications*, A volume in Micro and Nano Technologies, Elsevier, 2019.

SPECTROSCOPIC TECHNIQUES IN INORGANIC CHEMISTRY

L	T	P	C
3	0	0	3

CY527 **Scheme**

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Explore some spectroscopy techniques for inorganic compounds.
CO2	Study on applications of NMR spectroscopy in inorganic compounds.
CO3	Explain on electron spin resonance spectroscopy.
CO4	Gain knowledge on nuclear quadrupole resonance spectroscopy.
CO5	Differentiate on infrared and Raman Spectroscopy for inorganic compounds.

2. Syllabus:

- **NMR SPECTROSCOPY** **(10 Hours)**
  Use of Chemical shifts and spin-spin couplings for structural determination, Double resonance and dynamic processes in NMR, Decoupling phenomenon, Nuclear Overhauser Effect, DEPT spectra and structural applications in 13C NMR, Use of Chemicals as NMR auxillary reagents (shift reagents and relaxation reagents), 1H NMR of paramagnetic substances, NMR of Metal nuclei. Stereochemical non-rigidity and fluxionality: Introduction, use of NMR in its detection, its presence in trigonalbipyramidal molecules (PF_5), Systems with coordination number six ($Ti(acac)_2Cl_2$, $Ti(acac)2Br_2$, $Ta_2(OMe)_{10}$).

- **ELECTRON SPIN RESONANCE SPECTROSCOPY** **(08 Hours)**
  Basic principle, Hyperfine Splitting (isotropic systems); the **g** value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Electron-electron interactions, Anisotropic effects (the **g** value and the hyperfine couplings); Structural applications to transition metal complexes.

- **NUCLEAR QUADRUPOLE RESONANCE SPECTROSCOPY** **(08 Hours)**
  Basic concepts of NQR (Nuclear electric quadrupole moment, Electric field gradient, Energy levels and NQR frequencies), Effect of magnetic field on spectra, Factors affecting the resonance signal (Line shape, position of resonance signal) Relationship between electric field gradient and molecular structure. Interpretation of NQR data, Structural information of the following: PCl_5, $TeCl_4$, $Na(GaCl_4)$, BrCN, HIO_3 and Hexahalometallates.

- **MÖSSBAUER SPECTROSCOPY** **(08 Hours)**
  Basic principle, conditions for Mossbauer spectroscopy, Spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature dependent effects, structural deductions for iron and tin complexes, miscellaneous applications.

- **INFRARED AND RAMAN SPECTROSCOPY** **(08 Hours)**
  Applications of vibrational spectroscopy in investigating (i) symmetry and shapes of simple AB2, AB3 and AB4 molecules on the basis of spectral data, (ii) mode of bonding of ambidentate ligands (thiocyanate, nitrate, sulphate and urea). Distinction between Ionic and coordinate anions such as NO^{3-}, SO_4^{2-} and SCN^-, Lattice and coordinated water. Mode of bonding of ligands such as urea, dimethylsulphoxide and hexamethylphosphoramide.

(Total Lecture Hours: 42)

3. Books Recommended:

1. R. S. Drago, *Physical Methods in Inorganic Chemistry*, 4th Edition, Affiliated East-West Press, New Delhi, 2012.
2. G. Aruldhas, *Molecular Structure and Spectroscopy*, 2nd Edition, Prentice Hall of India Pvt. Ltd., New Delhi, 2001.
3. E. D. Olsen, *Modern Optical Methods of Analysis*, 1st Edition, McGraw-Hill Inc., US, 1975.
4. K. Nakamoto, *Infrared Spectra of Inorganic and Coordination Compounds*, 6th Edition, John Wiley & Sons, 2008.
5. D. N. Sathyanarayana, *Introduction to Magnetic Resonance Spectroscopy ESR, NMR, NQR*, 2nd Edition, I. K. International Publishing House Pvt. Ltd., 2009.

HETEROCYCLES AND ORGANIC SYNTHESIS

L	T	P	C
3	0	0	3

CY529 **Scheme**

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Discuss synthesis, reactivity and significance of various types of heterocycles.
CO2	Demonstrate the importance of microwave assisted synthesis over conventional methods.
CO3	Acquaint with synthetic strategies.
CO4	Analyze multicomponent reactions and discuss its advantage over traditional approach.
CO5	Explain synthesis, reactivity and significance of various types of heterocycles.

2. Syllabus:

- **FIVE AND SIX MEMBERED HETEROCYCLES WITH ONE AND TWO HETERO ATOMS** **(07 Hours)**
  Synthesis, reactivity, aromatic character and importance of following heterocyclic rings:, Pyrazole, Imidazole, Oxazole, Thiozole, Iosoxazole, Pyridine, Pyrimidine, Pyrazine, Oxazine and thiazine.

- **CONDENSED FIVE AND SIX MEMBERED HETEROCYCLES** **(07 Hours)**
  Synthesis, reactivity, aromatic character and importance of Benzofuran, Benzothiophene, Coumarins and Chromones, Condensed five membered heterocycles- Benzoxazole, Benzthiazole, Benzimidazole.

- **FIVE AND SIX MEMBERED HETEROCYCLES WITH MORE THAN TWO HETERO ATOMS** **(07 Hours)**
  Synthesis, reactivity, aromatic character and importance of following heterocycles:1,2,3-triazole, 1,2,4-triazole, 1,2,4- oxadiazole, 1,3,4- oxadiazole, 1,2,5- oxadiazole,tetrazole, 1,2,3-triazine, 1,2,4-triazine, 1,3,5-triazine,tetrazine, purines, pyrimidines and pteridines.

- **MICROWAVE ASSITED ORGANIC SYNTHESIS** **(07 Hours)**
  Microwave effect vs thermal effect, microwave reactors, reactions in homogeneous media and solvent, reactions of reagent supported on mineral acids, solvent free phase transfer catalysis.

- **MULTI-COMPONENT REACTIONS** **(06 Hours)**
  Relative reactivities of functional group to MCR, selected reactive functionalies in MCR like carbonyl, isocyanide; types of MCR, Diversity in MCR: Ugi, Passerini, Biginelli and Mannich reactions.

- **SYNTHETIC STRATGIES** **(08 Hours)**
  Reterosynthetic approach, Umpolung strategy, Ring formation reactions: Pausan- Khand, Bergman and Nazerov cyclization, Click chemistry: criterion for click chemistry, Enamines in Organic synthesis.

(Total Lecture Hours: 42)

3. Books Recommended:

1. J. A. Joule, K. Mills, *Heterocyclic Chemistry*, 5th Edition, Wiley Blackwell, 2010.
2. A. R. Katritzky, J. M. Lagowski, *The Priniciples of Heterocyclic Chemistry*, 1st Edition, Academic Press, 1968.
3. L. Kurti, C. Barbara, *Strategic Applications of Named Reactions in Organic Synthesis*, 1st Edition, Elsevier Academic Press, 2005.
4. T. J. J. Muller, *Science of Synthesis: Multicomponent Reactions,* Volume 1, 1st Edition, Thieme publishers, 2014.
5. D. Bogdal, *Microwave-assisted Organic Synthesis: One Hundred Reaction Procedures*, Volume 25, 1st Edition, Elsevier, 2005.

C-H FUNCTIONALIZATION

L	T	P	C
3	0	0	3

CY531 **Scheme**

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Acquire deep knowledge of advanced organometallic chemistry
CO2	Identify how these individual reactions make up a catalytic cycle
CO3	Appreciate C–H interactions with transition metals and how C–H activation can occur at a transition metal center.
CO4	Explain the role of photo catalysis in modern synthetic methodology
CO5	Propose the importance of catalysis in industrial processes.

2. Syllabus

- **Advanced Organometallic Chemistry of Transition Elements** **(18 Hours)**
  Introduction to the fundamentals of homogeneous catalysis and the mechanisms in organometallic chemistry: Oxidative addition, sigma bond metathesis, reductive elimination, insertion and elimination. Metal mediated C-C and C-X coupling reactions Heck, Negishi, Suzuki, and Stille, Sonogashira, Nozaki-Hiyama, Kumada, Buchwald-Hartwig, Catellani, Fujiwara-Moritani reactions and their synthetic utility in drug synthesis. Directed orthometalation, Metal (Pd, Rh) catalyzed C-H activation reactions and their synthetic utility, Copper and rhodium based carbene and nitrene complexes, Cyclopropanation, Rh catalyzed C-H insertion and aziridination reactions including asymmetric version, Noyori asymmetric hydrogenation. Introduction to N-heterocyclic carbene metal complexes. Tebbe's reagent, Pauson-Khand reaction, Hydroformylation, Carbonylation reactions.

- **C-H Bond Activation and Functionalization** **(14 Hours)**
  Interaction of metal centres with C-H bonds, agostic interactions and C-H activation, electrophilic and metalloradical activation. Organic synthesis involving chelation-assisted C-H activation, *ortho*-C-H activation, Distal C-H activation, C-H activation in heterocycles synthesis. C-H, C=C and C≡C activated annulation reactions. Important synthetic approaches *via* C-X (X= C, N, O, S etc.) bond activation. Role of non-metallic activation of bonds in organic synthesis.

- **Visible Light Photocatalysis in Organic Chemistry** **(10 Hours)**
  Introduction, Basics of the photocatalytic cycle, Generation of radicals, C—X (X = N, O, S etc.) bond formation, C-C bond formation, Atom transfer radical addition reactions, Cycloaddition reactions, Arene functionalization, Application of visible-light-mediated reactions to the synthesis of pharmaceutical compounds.

(Total Lecture Hours: 42)

3. Books Recommended:

1. A. Yamamoto, *Organotransition Metal Chemistry, Fundamental Concept and Applications*, 1st Edition, John Wiley, 1986
2. R.H. Crabtree, *The Organometallic Chemistry of Transition Metals*, 2nd Edition, John Wiley, 1994
3. D. W. C. MacMillan, *Visible Light Photocatalysis in Organic Chemistry*, 1st Edition, John Wiley, 2018

4. J. Yu Z. Shi, *C-H Activation (Topics in Current Chemistry Book 292)*, 1st Edition, Springer, 2010
5. J. Yu, *Science of Synthesis: Catalytic Transformations via C-H Activation*, Volume 1, 1st Edition, Thieme, 2016.

SUPRAMOLECULAR CHEMISTRY

L	T	P	C
3	0	0	3

CY533

Scheme

1. Course Outcomes (COs):

At the end of the course the students will be able to:

CO1	Acquire basic and need of supramolecular chemistry.
CO2	Study on thermodynamic and kinetic aspects of host-guest chemistry.
CO3	Gain advance knowledge on artificial host molecules.
CO4	Explain molecular self-assembly.
CO5	Explore the application of supramolecular chemistry in device fabrication.

2. Syllabus

- **FUNDAMENTALS OF SUPRAMOLECULAR CHEMISTRY** **(06 Hours)**
  Molecules, super molecules and supramolecular Chemistry, non-covalent interactions, complementarity and cooperativity, supramolecular chemistry of life.

- **HOST-GUEST CHEMISTRY** **(14 Hours)**
  Host-guest complexation, Thermodynamics of host-guest complexation, Molecular recognition – factors involved, Molecular receptors/ Ionophores – design principles; Molecular receptors for cations, anions and neutral molecules, Crown ethers, cryptands, spherands, cyclodextrins, cucurbituril, and calixarenes, cavitands, molecular clips, clefts and tweezers, Threading of a linear molecule through a cyclic molecule, Creation of rotaxanes and catenanes.

- **SELF-ASSEMBLY** **(12 Hours)**
  Biological self-assembly, self-assembly in synthetic systems, self-assembling coordination compounds, capsules, helicates and molecular knots, organic and inorganic nanomaterials, Crystal nucleation and growth, understanding crystal structures, supramolecular gels, supramolecular polymers, Amphiphiles and their aggregation, Aggregation induced emission and quenching.

- **MOLECULAR DEVICES** **(10 Hours)**
  Supramolecular photochemistry and devices, chemosensors, molecule-based electronics: Molecular wires, molecular switches, molecular logic, molecular rectifiers and molecular electronic devices.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. J. W. Steed, J. L. Atwood, *Supramolecular Chemistry*, 2nd Edition, John Wiley, 2009.
2. K. Ariga, T. Kunitake, *Supramolecular Chemistry, Fundamentals and Applications*, 1st Edition, Springer, 2006.
3. J. W. Steed, D. R. Turner, K. J. Wallace, *Core Concepts in Supramolecular Chemistry and Nanochemistry*, 1st Edition, Wiley, 2007.
4. H. Dodziuk, *Introduction to Supramolecular Chemistry*, Springer, 1st Edition, 2002.
5. J. M. Lehn, *Supramolecular Chemistry*, 1st Edition, Wiley-VCH, 1995.

PHYSICAL METHODS OF STRUCTURE DETERMINATION

L	T	P	C
3	0	0	3

CY535

Scheme

1. Course Outcomes (Cos):

At the end of the course students will be able to:

CO1	Explain fundamentals of crystal growth and crystal habits.
CO2	Acquire profound knowledge in crystal systems.
CO3	Execute X-ray crystallographic knowledge for solving structures.
CO4	Enumerate the spectral behaviour of a molecule with unpaired electrons.
CO5	Interpret magnet properties of a molecule.

2. Syllabus:

- **CRYSTAL GROWTH** **(08 Hours)**

  Nucleation phenomenon – Homogenous and Heterogeneous nucleation, Theories of crystal growth. Defects, Classification of crystal growth methods: Melt, solution and Vapour Growth Techniques. Crystal habits and aggregates.

- **CRYSTAL STRUCTURE** **(20 Hours)**

  Crystal symmetry, Cell parameters and Crystal systems, Cubic crystal system & lattices; Density & Packing Fraction; Miller indices of crystallographic planes & directions; interplanar distance, Determination of crystal structure using X-ray diffraction techniques viz. Laue method, rotating crystal method (Bragg method) & powder method. X-ray Diffraction pattern of a cubic system: Indexing of powder diffraction patterns. Coordinates of Points, Structure factor calculation, Diffraction Intensity, preparation of structure plots including ORTEP and lattice structures including packing diagrams. Crystal packing and **Visualisation through MERCURY and DIAMOND software,** diffractometer instrumentation, Practical exercise of structure determination using standard packages. Basic Refinement exercise.

- **EPR SPECTROSCOPY AND MAGNETIC PROPERTIES** **(14 Hours)**

  Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants spin Hamiltonian, spin densities and Mc Connell relationship, applications. Structure characterization of Cu(II) complexes using EPR spectroscopy, Isotropic, axial and rhombic EPR spectra and interpretation.

  Magnetic properties -Determination of Magnetic moments and their applications to the elucidation of structures of inorganic compounds – temperature independent paramagnetism, Field-dependent magnetization, Magnetic properties of transition metals. Spin crossover in coordination compounds – Single molecule magnets, Plotting MPMS Data.

(Total Lecture Hours: 42)

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3. Books Recommended:

1. M. M. Woolfson, *An Introduction to X-ray Crystallography*, 2nd Edition, Cambridge University Press; 1997.
2. J. C. Brice, *Crystal Growth Processes*, John Wiley and Sons, New York, 1986
3. J. W. Mullin, *Crystallization*, 4th Edition, Elsevier Butterworth-Heinemann, London, 2001.

4. A. W. Vere, *Crystal Growth: Principles and Progress*, 1st Edition, Plenum Press, New York, 1987.
5. R. S. Drago, *Physical Methods in Inorganic Chemistry*, 2nd Edition, International Edition East-West Press, 2016.

FIFTH YEAR OF FIVE YEARS INTEGRATED M. Sc. (CHEMISTRY)
M. Sc. - V, SEMESTER – X

Sr. No.	Subject	Code	Scheme	Credit	Examination Scheme				Total Marks
					Theory	Tutorial	Practical		
							Int.	Ext.	
1.	Dissertation	CY-502	0-0-24	12	00	00	160	240	400
Total contact hours per week=24			**Total Credits=12**			**Total Marks=400**			

Total hours: 280 Total Credits: 212

On Successful Completion of the course, the candidate will be awarded 5-Years Integrated M. Sc. Degree in Chemistry.