MANONMANIAM SUNDARANAR UNIVERSITY

DEPARTMENT OF CHEMISTRY

STRUCTURE OF M.Sc. CHEMISTRY PROGRAM

For the academic year 2021-2022

Preamble

The emerging Chemical Technologies are highly science based. A Chemist cannot isolate himself from other disciplines. The practice of Chemistry over a span of more than a century has created unavoidable impacts of human environment. The adverse effects were particularly noted during last few decades. The concept of sustainable development is now well accepted. The principles and applications of Chemistry should be learnt on this background.

Necessity

The purpose of post-graduate education in Science is to create highly skilled manpower in specific areas, which will lead to generation of new knowledge and creation of wealth for the country. Chemistry is a fundamental science and has contributed immensely to the improvement of the life of human beings by providing many of human requirements and essentialities.

Importance

Chemistry is important to the world economy as well. The developments in Chemistry during last few decades are phenomenal. It is also seen that these developments are crossing the traditional vertical boundaries of scientific disciplines; the more inclination is seen towards biological sciences. New branches of Chemistry are emerging and gaining importance, Such as bioorganic chemistry, Materials chemistry, computational chemistry etc. The practice of Chemistry at industrial scale also is undergoing radical changes and is more or more based on deep understanding the chemical phenomena.

Objectives

i. To impart training in Chemistry at advanced level in a more holistic way and enthuse the students for the subject.
ii. To train the students to make them confident and capable of accepting any challenge in Chemistry.
iii. To give a flavour of research in Chemistry and train the students for research career.
iv. To abreast the students about the current status and new developments in Chemistry.

v. To make the students aware of the impact of Chemistry on environment and imbibe the concept of sustainable developments.

vi. To educate the students with respect to skills and knowledge to practice chemistry in way that are benign to health and environment.

Outcome

After completing the M.Sc. program the students will be able to

i. Pursue research program

ii. Qualify as Chemist/Scientist in various industries and research institutions

Eligibility Norms

B.Sc. degree in Chemistry or any other equivalent Bachelor Degree is eligible for the admission in M.Sc. Chemistry program.

Scheme of Examination and question pattern

Time: 3 hours Max. marks:75

Part A	:	10 questions full of Objective type WITHOUT multiple choice. Two questions from each unit of a paper. Each question carries one mark	10 x 1=10 marks
Part B	:	5 descriptive questions, of either a or b type (internal choice). One question is from each unit. Each question carries 5 marks	5 x 5 = 25 marks
Part C	:	5 descriptive questions of either a or b type (internal choice). One question is from each unit. Each question carries 8 marks.	5 x 8 = 40 marks

Course Weight:

In each of the courses, credits will be assigned on the basis of the lectures, tutorials / lab work and other forms of learning in a 15 week schedule.

1. One credit for each lecture hr. per week
2. One credit for each tutorial hr. per week
3. One credit for every two hrs. of Lab or Practical Work per week

Internal /External Distribution of Marks

For all theory papers, the Internal / External distribution of Mark will be 25: 75 (Total = 100).

The 25 marks for the Internal component has been divided as follows:

3 compulsory tests, out of which average of the best two tests	= 15 marks
Seminar	= 5 marks
Assignment	= 5 marks
Total	=25 marks

For all Practical papers the examination time shall be 6 hours and the Internal / External distribution of Marks will be 50: 50 (Total = 100) respectively.

Internal component of 50 marks is divided as follows:

For the regular class periodical assessment	= 25 marks
2 Compulsory Internal test,	
Out of which Average of two internal test	= 25 marks
Total	=50 marks

External Examination:

Record	= 10 marks
Practical Examination	= 40 marks
Total	=50 marks

There is no internal passing minimum. There is a passing minimum of 50% for external and overall components.

PROJECT

Project for IV semester shall be an INDIVIDUAL project. Project evaluation will be done by Guide and another faculty member of the department. Viva voce Examination for the project students will be conducted jointly by the same examiners who evaluated the project report.

Course Structure of M.Sc Chemistry Program

The credit and teaching norms of the program is distributed as under.

Sl. No.	Subject Code	Subject Name	Credits	Hrs./ week
		I Semester		
1	NCHC11	Concepts of Organic Chemistry	4	4
2	NCHC12	Inorganic Bonding & Reaction mechanism	4	4
3	NCHC13	Quantum Mechanics	4	4
4	NCHCPA	Thermodynamics (e- learning course)	4	4
5	NCHCEA-NCHCEF	Elective Paper	3	3
6	NCHL11	Organic Chemistry Practical- I	2	4
	NCHL12	Organic Chemistry Practical– II	2	4
		Total	**23**	**27**
		II Semester		
7	NCHC21	Reaction and Mechanism of Organic Chemistry	4	4
8	NCHC22	Organometallic Chemistry	4	4
9	NCHC23	Analytical Chemistry	4	4
10	NCHC24	Group Theory and Spectroscopy	4	4
11	MOOC	Supportive course paper I	3	3
12	NCHL21	Physical Chemistry Practical I	2	4
	NCHL22	Physical Chemistry Practical – II	2	4
		Total	**23**	**27**
		III Semester		
13	NCHC31	Organic Synthesis	4	4
14	NCHC32	Electrochemistry	4	4
15	NCHC33	Bio-inorganic chemistry	4	4
16	NCHC34	Principles and applications of Spectroscopy	4	4
17	MOOC	Supportive course Paper II	3	3
18	NCHL31	Inorganic Chemistry Practical – I	2	4
	NCHL32	Inorganic Chemistry Practical– II	2	4
		Total	**23**	**27**
		IV Semester		
19	NCHEPB	Elective Paper – II (e- learning course)- Photochemistry & Surface	3	3
20	NCHCEA-NCHCEF	Elective Paper – III	3	3
21	NCHL41	Advanced Organic practical	2	4
22	NCHL42	Advanced Inorganic Practical	2	4
23	NCHL41	Advanced Physical Practical	2	4
24	NCHP41	Project	9	12
		Total	**21**	**30**
		Grand Total	**90**	**111**

SEMESTER - I

Concepts of Organic Chemistry

L (hrs)	Credit
60	4

Objectives

1. To study the chemical bonding and structure of molecules
2. To study the mechanism of reactions
3. To understand the concept of Aromaticity and stability of molecules
4. To know about the Stereochemistry of molecules
5. To understand the concept of asymmetric synthesis of organic molecules

Unit I Chemical Bonding and Structure (12 hrs.)

Review of basic principles of structure and bonding, application of acid base concepts, Inductive effect – Mesomeric effect – Steric Inhibition of resonance – '$p\pi$-$d\pi$' bonding – hyperconjugation – cross conjugation – hydrogen bonding - acidity, basicity, factors affecting the strength of acids and bases - HSAB theory. Generation, structure, stability and reactivity of carbocations, carbanions, free radicals, carbenes and nitrenes. Effect of structure on reactivity.

Unit II Reaction Mechanism (12 hrs.)

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, Hammond postulate, Microscopic reversibility, Curtin-Hammett principle, transition states and intermediates, methods of determining mechanisms, isotopic effects. The Hammett equation and linear free energy relationship (sigma-rho) relationship, Taft equation.

Unit III Aromaticity: (12 hrs.)

Aromaticity and antiaromaticity, Hückel's rule, non-aromaticity, anti-aromaticity, homo-aromaticity n-annulenes, heteroannulene, fullerenes, C-60, cryptates, Bonds weaker than covalent; addition compounds, inclusion compounds, crown ethers, cyclodextrins, catenanes and rotaxanes.

Unit IV Stereochemistry (12 hrs.)

Conformational analysis of cycloalkanes, effect of conformation on reactivity. Elements of symmetry, chirality, molecules with more than one chiral center, projection formulae (i) Fischer (ii) Sawhorse (iii) Newman (iv) Flying Wedge; threo and erythro isomers, methods of resolution, optical purity, enantiotopic and diastereotopic atoms, groups and faces, stereospecific and stereoselective synthesis. Optical activity in the absence of chiral carbon-Biphenyl, allene and spiranes.

Unit V Asymmetric Synthesis (12 hrs.)

Chiral auxiliatries, methods of asymmetric induction – substrate, reagent and catalyst controlled reactions; determination of enantiometric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic. Cram's rule, Prelog's rule - stereoselective and stereospecific synthesis.

Asymmetric reactions with mechanism: Aldol and related reactions including Cram's rule, Sharpless enantioselective epoxidation, hydroxylation, amino hydroxylation, Diels-Alder reactions.

References

1. F. A. Carey and R. A. Sundberg, Advanced Organic Chemistry, Part A: Structure and Mechanisms, 5th Edition, Springer, New York, 2007.
2. Stereochemistry of Carbon Compounds by E. J. Eliel, McGraw Hill
3. Organic Chemistry by S. H. Pine, McGraw Hill,1987
4. Stereochemistry of Organic Compounds by D. Nasipuri, Wiley,1994.
5. Robert E. Gawley, Jeffrey Aube, Principles of Asymmetric Synthesis, pergamon, 2nd edition, 1996
6. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 2002.
7. Stereochemistry, D. G. Morris, , RSC Tutorial Chemistry Text 1, 2001.
8. E. L. Eliel and S. H. Wilen, Stereochemistry of Organic Compounds, John Wiley & Sons, New York, 1994.
9. D. G. Morris, Stereochemistry, RSC Tutorial Chemistry Text 1, 2001
10. J. Kirby, Stereoelectronic effects, Oxford Chemistry Primers, 2011.
11. Steric and Stereoelectronic Effects in Organic Chemistry, V. K. Yadav, Springer, 2016.

Inorganic Bonding & Reaction mechanism

Objectives

L (hrs)	Credit
60	4

1. To provide advanced concepts about bonding reactions and redox potentials of inorganic compounds
2. To introduce bonding concepts, magnetic spectra and optical behavior of coordination complexes
3. To disseminate knowledge on reaction mechanism of coordination complexes.

Unit I Carboranes and silicates (12 hrs.)

Synthesis, Properties, structure and bonding of: Pseudo halogen, Interhalogen and Xenon compounds, Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates.

Unit II Acid & Base (12 hrs.)

Redox Reactions: Latimer diagram, Electrochemical Series. Acids and Bases: Lewis acids and bases; HSAB concept. Transition Metal Chemistry: Nomenclature, Isomerism, Chelate effect, Macrocyclic ligands, thermodynamic stability, successive and overall stability constants, Irving-William series.

Unit III Structure & Bonding (12 hrs.)

Bonding in Coordination Complexes: VSEPR theory, Crystal-Field theory, d-orbital Splitting in Octahedral, Tetrahedral, Square Planar geometries; Molecular Orbital Theory, p-bonding; Jahn-Teller effect, Spectrochemical series, nephelauxetic series. Electronic Spectra: d-d transitions, Orgel diagrams, charge-transfer spectra.

Unit IV Reaction Mechanism (12 hrs.)

Substitution reaction in octahedral and square planar complexes; lability, trans-effect, Conjugate base mechanism, racemisation, Electron Transfer Reactions: inner sphere and outer sphere mechanism, application of electron transfer reaction in synthesis of coordination complexes.

Unit V Electronic Spectra (12 hrs.)

UV-Vis, charge transfer, colors, intensities and origin of transitions, interpretation, term symbols and splitting of terms in free atoms, selection rules for electronic transitions, calculation of Dq, B, C, Nephelauxetic ratio.

Magnetism: Types, determination of magnetic susceptibility, spin-only formula, spin-orbit coupling, spin crossover.

References

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed. Pearson education, 2006.
2. Concepts and Models of Inorganic Chemistry by B. E. Douglas, D.H. Mc Daniel and J. J. Alexander, John Wiley, 1994, 3rded.
3. Physical Inorganic Chemistry: A Coordination Chemistry Approach by S.F.Kettle, Spektrum,1999, Oxford press.
4. Chemistry of the Elements by N. N. Greenwood and A. Earnshaw, Pergamon, Reprinted 2005.
5. Advanced Inorganic Chemistry by F. A. Cotton, G. W. Wilkinson, 5thedition, John-Wiley & Sons,1999.
6. Physical Methods in Chemistry by R. S. Drago, Saunders,1992
7. Inorganic Electronic Spectroscopy by Edward 1.Solomon and A.B.P. Lever, Johnwiley & sons,2006.
8. Introduction to Magneto chemistry by A. Ernshaw, Academic press, 2013.

Thermodynamics (e- learning course)

Objectives

L (hrs)	Credit
60	4

1. To understand the concept of chemical equilibrium and kinetics of reactions
2. To learn about the heat exchange and thermodynamics of reactions
3. To study about the electrical properties of ions in solutions

Unit I Fundamental concepts of thermodynamics (12 hrs.)

Fundamental equations for open systems, Partial molar quantities and chemical potential, Chemical equilibrium, Phase behavior of one and two component systems, Ehrenfest classification of phase transitions.

Unit II Statistical Thermodynamics (12 hrs.)

Introduction, Concept of ensembles, partition functions and distributions, microcanonical, canonical and grand canonical ensembles, canonical and grand canonical partition functions, Boltzmann, Fermi-Dirac and Bose-Einstein distributions.

Unit III Thermodynamics of Ideal gases (12 hrs.)

Canonical partition function in terms of molecular partition function of non-interacting particles, Heat capacity (Cv, Cp) of an ideal gas of linear and nonlinear molecules, chemical equilibrium.

Unit IV Thermodynamics of Real gases (12 hrs.)

Canonical partition function for interacting particles, intermolecular potential (Lennard-Jones, Hard-sphere and Square-well) and virial coefficients. Temperature dependence of the second virial coefficient.

Unit V: Thermodynamics of solids & Metals (12 hrs.)

Solids: - Einstein and Debye models. T^3 dependence of heat capacity of solids at low temperatures (universal feature).

Metals: Fermi function, Fermi energy, free electron model and density of states, chemical potential of conduction electrons.

References

1. P. Atkins and J. Paula, Physical Chemistry, 10th Edition, Oxford University Press, Oxford,2014.
2. D. A. Mc Quarrie and J. D. Simon, Molecular Thermodynamics, University Science Books, California 2004.
3. R. S. Berry, S. A. Rice and J. Ross, Physical Chemistry, 2nd Edition, Oxford University Press, Oxford, 2007.
4. D. A. Mc Quarrie, Statistical Mechanics, University Science Books, California 2005
5. B. Widom, Statistical Mechanics - A Concise Introduction for Chemists, Cambridge, University Press, 2002.
6. S. Glasstone, Text Book of Physical Chemistry, 2nd Edition, Macmillan India Ltd, New Delhi , 1974.
7. e-PG Pathshala- P-06- Physical Chemistry.

Quantum Mechanics

L (hrs)	Credit
60	4

Objectives

1. To study about the quantum mechanics of the molecules
2. To understand the concept of MO theory and VB theory
3. To study about the representations and eigen values.

Unit I Quantum Mechanics – I (12 hrs.)

Postulates of quantum mechanics, Hermitian operators, Commutators and results of measurements in Quantum Mechanics. Eigen functions and eigen values of operators.

Unit II Quantum Mechanics – II (12 hrs.)

Solution of the Schrodinger equation for exactly solvable problems for bound states such as particle-in-a- box.

Unit III Advanced topics and Atomic Spectra (12 hrs.)

Harmonic oscillator and rigid rotor, Solution of the Schrodinger equation for the hydrogen atom, radial and angular probability distributions, atomic orbitals and electron spin.

Unit IV Approximation methods-Perturbation theory and variation theorem (12 hrs)

Born-Oppenheimer approximation, VB and MO theory, H_2^+, H_2 molecule problem, Hückel molecular orbital theory and its application to ethylene, butadiene and benzene.

Unit V Time dependent Mechanics (12 hrs.)

The time dependent Schrödinger equation. Co-ordinate and momentum space representation of operators and eigen states; Schrodinger and Heisenberg representations.

References:

1. E. Kreyszig, Advanced Engineering Mathematics, 5th edition, Wiley Eastern, 1989.
2. G. Arfken and Hans J. Weber, Mathematical methods for physicists, Prism Indian Edition,1995.
3. D. A. McQuarrie, Quantum Chemistry, University Science Books,1983.
4. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition, Oxford University Press,1983.

5. N. Levine, Quantum Chemistry, 3rd edition, Allyn and Bacon,1983.
6. D. J. Griffiths, Introduction to Quantum Mechanics, Pearson Education,2005.
7. H. Kuhn, H.-D. Försterling, and D.H. Waldeck, Principles of Physical Chemistry, 2nd edition, Wiley,2009.
8. J. P. Lowe, Quantum Chemistry, K. A. Peterson, 3rd edition, Academic Press, 2006.
9. e-PG Pathshala – P-02- Physical Chemistry- I (Quantum Chemistry)

ORGANIC CHEMISTRY PRACTICAL – I

Objective

To know about the basic concept and to improve the practical knowledge of the students.

P (hrs)	Credit
60	2

Practicals

1. Single stage preparations:

   Diels – Alder Reactiom, Bis – 2 – Naphthol, 1,2,3,4 – Tetrahydrocarbazole, Benzpinacol, Benzpinacolone, Aspirin, Phenol – formaldehyde resin, p – Nitroacetanilide, β – D – Glucopyranose, Fluorescein, p - Bromoacetanilide
2. Two stage preparation:

   Synthesis of Phthalamide, p – nitroaniine, p – Bromo aniline, M – nitrobenzoic acid

References

1. I. Vogel, A Text Book of Practical Organic Chemistry, 1989.
2. Ault, Techniques and Experiments for Organic Chemistry, 1998.
3. N. K. Vishnoi, Advanced Practical Organic Chemistry, 1979.
4. B. Dey and M.V. Sitaraman, Laboratory Manual of Organic Chemistry, 2017.
5. Raj K. Bansal, Laboratory Manual in Organic Chemistry, 1994.

ORGANIC CHEMISTRY PRACTICAL – II

Objective

To understand the basic concept and to enhance the technical skill of the students.

P (hrs)	Credit
60	2

Practicals

1. Separation and systematic analysis of Organic binary mixtures.
2. Estimation of phenol, aniline, methyl ethyl ketone, glucose.

References

1. I. Vogel, A Text Book of Practical Organic Chemistry, 1989.
2. Ault, Techniques and Experiments for Organic Chemistry, 1998.
3. N. K. Vishnoi, Advanced Practical Organic Chemistry, 1979.
4. B. Dey and M.V. Sitaraman, Laboratory Manual of Organic Chemistry, 2017.
5. Raj K. Bansal, Laboratory Manual in Organic Chemistry, 1994.

SEMESTER - II

Reaction& Mechanism of Organic Chemistry

Objectives

L (hrs)	Credit
60	4

1. To study about the Aliphatic and aromatic nucleophilic substitution reactions
2. To study about the Aliphatic and aromatic electrophilic substitution reactions
3. To understand the concept of Free radical reactions
4. To know about the concept of substitution and addition reactions
5. To learn about the concept of elimination reactions

Unit I Nucleophilic Substitution (12 hrs.)

Aliphatic Nucleophile Substitution : The SN^2, SN^1, mixed SN^1 and SN^2 and SET mechanisms. The neighbouring group mechanism. Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements.The SN^i mechanism. Nucleophilic substitution at an allylic, aliphatic trigonal and a vinyl carbon. Reactivity effects of substrate structure, attaching nucleophile, leaving group and reaction medium.

Aromatic Nucleophile Substitution: The SNAr, SN^1, benzyne and SRN^1 mechanisms. Reactivity; effect of substrate structure, leaving group and attacking nucleophile.

Unit II Electrophilic Substitution (12 hrs.)

Aliphatic: Bimolecular mechanisms: SE^1, SE^2 and SE^i. The SE^1 mechanism, electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity. Aromatic: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles .

Unit III Free Radical Reactions (12 hrs.)

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridge head. Reactivity in the attaching radicals. The effect of solvents on reactivity.

Unit IV Addition to Carbon-Carbon Multiple Bonds **(12 hrs.)**

Mechanistic and stereo chemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemo-selectivity, orientation and reactivity. Addition to cyclopropane ring. Hydroboration. Addition to Carbon-Hetero Multiple Bonds: Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles.

Unit V Elimination Reactions **(12 hrs.)**

The E^2, E^1 and E^1CB mechanisms and their spectrum. Orientation of the double bond. Reactivity effects of substrate structures, attaching base, the leaving group and the medium.

References

1. Advanced Organic Chemistry by J. March, John Wiley & Sons,1992
2. Organic Chemistry by S. H. Pine, Mc Graw Hill,1987.
3. Modern Synthetic Reactions by H. O. House, W.A. Benjamin, Inc.,1972
4. Understanding Organic Reaction Mechanism by A. Jacobs, Cambridge 1998.
5. Organic Chemistry by J. M. Horn back, Books Coley, 1998.
6. Organic Chemistry by P.Y. Bruice, Prentice Hall, 1998.
7. Organic Reaction and their Mechanism by P.S. Kalsi, New Age, 1996.

Organometallic Chemistry

L (hrs)	Credit
60	4

Objectives

1. To study about the Classification of Organometallic compounds
2. To study about the elimination and insertion reactions
3. To know about the importance of Catalyst
4. To Understand the concept of polymerization process.
5. To learn about the fundamental process of transition metal complexes.

Unit I Metal carbonyl & Nitrosyl (12 hrs.)

Definition, classifications and bonding in organometallic compounds. EAN rule and its correlation to stability of organometallic compounds - synthesis, structure and bonding of metal carbonyls, nitrosyls and dinitrogen complexes; IR spectral characterization of carbonyls and nitrosyls - pi – acceptor complexes with alkene, alkyne, allyl, arene systems

Unit II Reaction Mechanism of organometallic compound (12 hrs.)

Substitution reactions of carbonyls; oxidative addition and reductive elimination, insertion and elimination reactions; nucleophilic and electrophilic attack of coordinated ligands; addition to bimetalic species and cyclometallation reactions. Metallocenes; synthesis, properties, structure and bonding with particular reference to ferrocene and berryllocene.

Unit III Organometallic catalysis – I (12hrs.)

Organometallic catalysts and the requirements; Terminology in catalysis, Turnover, Turnover number (TON), turnover frequency (TOF). Wilkinson's catalyst and hydrogenation reactions, Tolman's catalytic loop; hydroformylation (oxo) reaction, Wacker and Monsanto acetic acid processes. Cluster compound, polymer-supported catalyst.

Unit IV Organometallic catalysis – II (12hrs.)

Water gas shift reactions; Fischer Tropsch process and synthetic gasoline, The Heck Reaction, C-C coupling reaction, Suzuki process, The Stille Reaction, Oligomerizations, Lanthanoidocene Catalysts. Ziegler-Natta polymerization and mechanism of stereoregular polymer synthesis, olefin metathesis and metathesis polymerization

Unit V S-block Organometallics **(12 hrs.)**

S-block organometallic compounds: synthesis, structure and bonding of organo-lithium, beryllium and magnesium compounds.

Spectroscopic techniques in Organometallic chemistry. Electronic and magnetic properties of Organometallic compounds. Stoichiometric and catalytic reactions. Fundamental processes in reactions of organo-transition metal complexes.

References:

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th Ed. Harper Collins 1993. (See Pg:7)
2. Concepts and Models of Inorganic Chemistry by B. E. Douglas, D.H. McDaniel, J. J. Alexander, John Wiley, 1993, 3rdEd. (See Pg:8)
3. Reaction Mechanism of Inorganic Chemistry and Organometallic system by R. R. Jordan Oxford Univ. Press, 2007. 2ndEd.
4. Advanced Inorganic Chemistry by F. A. Cotton and G. W. Wilkinson, John- Wiley & Sons, 1988, 5thEd. (See Pg:8)
5. Organometallics by Ch. Elschenbroich, VCH, 2006, 3rd Ed.
6. Organotransition Metal Chemistry: Fundamental Concepts and Applications by A. Yamamoto, John Wiley1986.
7. Organometallic Chemistry of the Transition Metals by R. H. Crabtree, John.John Wiley& Sons, April 11, 2014.

Analytical Chemistry

Objectives

L (hrs)	Credit
60	4

1. To study about the Errors and Data Analysis
2. To study about the Advanced techniques in chromatography
3. To know about the electroanalytical techniques
4. To Understand about the surface techniques

Unit I Statistics for analytical experimentation (12 hrs.)

Probability, Regression analysis, Accuracy and propagation of errors, Data analysis. Mean, standard deviation, least square fit, testing the fit (C_2 test, residual etc.). Signal to noise ratio.

Unit II Advanced chromatographic techniques (12 hrs.)

Theory of separation methods: HPLC, GC, GC/MS, LC/MS, GPC, Supercritical fluid chromatography, Detectors in Chromatography, Applications of chromatography.

Unit III Electroanalytical techniques (12 hrs.)

Principles and analytical experimentation of Potentiometry, Electrogravimetry, Voltammetry, Stripping methods, Chronoamperometry, Quantitative applications of potentiometry and voltammetry, amperometric titrations.

Unit IV Atomic absorption and emission spectroscopy (12 hrs.)

Principles and applications of Fluorimetry, nephelometry, turbidimetry, Dynamic light scattering. Preliminary analyses of a spectrum: Relative populations of species from intensity, relate line widths to lifetime, Introduction to spectroscopy in time domain, Time-correlated single photon counting.

Unit V Surface Techniques (12 hrs.)

Principles and applications of Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), X-ray Photoelectron spectroscopy (XPS),electron spectroscopy for chemical analysis (ESCA), and Scanning Probe Microscopy.

References

1. D. A. Skoog, F. J. Holler and S. R. Crouch, Principles of Instrumental Analysis, 6th Edition, Brooks/Cole Cengage Learning, Belmont, CA,2007
2. H. H. Willard, L. L. Merrln, Jr., J. A. Dean, and F. A. Senle, Jr., Instrumental Methods of Analysis: Wadsworth, 7th Edition, Belmont.,1989
3. F. Rousseac and A. Roessac, Chemical Analysis: Modern Instrumentation Methods and Analysis, 4th Edition, John Wiley & Sons, Ltd.,2000
4. B. Voigtlaender, Scanning Probe Microscopy: Atomic Force Microscopy and Scanning Tunneling Microscopy:, Springer - Verlag, Berlin 2015.

Group Theory and Spectroscopy

L (hrs)	Credit
60	4

Objectives

1. To study about the Concept of Group theory
2. To study about the Application of group theory
3. To know about the Selection rules in spectroscopy
4. To Understand about the NMR, NQR, ESR Spectroscopic techniques

Unit I Molecular symmetry and Symmetry groups (12 hrs.)

Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct product representation.

Unit II Application of group theory (12 hrs.)

Application of group theory to normal mode analysis –symmetry selection rules for IR and Raman active fundamentals; symmetry of molecular orbitals and symmetry selection rule for electronic transitions in simple molecules (ethylene, formaldehyde and benzene); projection operators – SALC procedure – evaluation of energies and MO's for ethylene, butadiene and cyclopropenyl systems – application of group theory to solve hybridization problems.

Unit III Molecular Spectroscopy- I (12 hrs.)

Classification of molecules, rigid rotor model, selection rules, intensity of spectral lines, effect of isotopic substitution. Stark effect. Infrared: Review of harmonic oscillator, selection rules, vibrational energy of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R, branches. Breakdown of Born-Oppenheimer approximation, vibration of polyatomic molecules.normal mode of vibration, group frequencies, overtone, hot bands.

Unit IV Molecular Spectroscopy- II (12 hrs.)

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

Classical and quantum theories of Raman effect, pure rotational, vibrational and vibrational- rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman. Molecular Spectroscopy: Energy levels, MO, vibronic transitions, Franck- Condon principle, electronic spectra of polyatomic molecules. Emission spectra, radiative and non-radiative decay, internal conversion

Unit V Spin resonance Spectroscopy (12 hrs.)

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

NQR spectroscopy – principles- experimental set up- nuclear quadrupole coupling in atoms and molecules – applications.

ESR spectroscopy – basis principles – hyperfine splitting – origin of hyperfine interaction – the g value – McConnel relationship – applications of ESR.

References

1. Chemical Applications of Group Theory by F.A. Cotton, Wiley Interscience, 1990, 3rdEd.
2. Fundamentals of Molecular Spectroscopy by C. N. Banwell and E.M. Mc Cash, Tata McGraw Hill, 1994.
3. Group Theory and Quantum Mechanics by M. Tinkham, McGraw Hill,1964.
4. Introduction to Molecular Spectroscopy by G. M. Barrow, McGrawHill,1962.
5. Introduction to Atomic Spectra by H. E. White, McGraw Hill,1934.
6. Modern Molecular Photochemistry by Nicholas J. Turro, University Science Books,1991.
7. P. W. Atkins, Molecular Quantum Mechanics, 2nd edition, Oxford University Press,1983.
8. P. F. Bernath, Spectra of Atoms and Molecules, 2nd Edition, Oxford University Press,2005.
9. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders, 1997.

PHYSICAL CHEMISTRY PRACTICAL – I

P(hrs)	Credit
60	2

Objectives

1. To understand the basic concept of conductivity of ions
2. To study about the distribution of molecule between two phases
3. To know about the chemical kinetics of acid hydrolysis and salt effect

Practicals

Part 1: Conductivity

a. Determination of cell constant
b. Dissociation constant of a weak acid
c. Conductometric titrations:
   i. Estimation of HCl and AcOH in a mixture
   ii. Estimation of NH_4Cl and HCl in a mixture
   iii. Estimation of AcOH and Sodium acetate in a buffer

Part 2: Distribution law

a. Partition coefficient of Iodine between two immiscible solvents.
b. Study of the equilibrium constant of the reaction $KI + I_2 \rightarrow KI_3$

Part 3: Kinetics (atleast one)

a. Acid hydrolysis of ester – comparison of strength of acids.
b. Kinetics – persulfate – Iodide – clock reaction-primary salt effect.

References:

1. W. J. Popiel, Laboratory Manual of Physical Chemistry, ELBS, London 1970
2. Findlay's Practical Physical Chemistry, B. P. Levitt, Longman, London, 1985
3. S. K. Sinha, Physical Chemistry A Laboratory Manual, Narosa Publishing Pvt, Ltd., 2014.

PHYSICAL CHEMISTRY PRACTICAL – II

P (hrs)	Credit
60	2

Objectives

1. To understand the concept of solubility product, dissociation constant and Potentiometry titrations
2. To study about the physical and chemical behavior of oxalic acid on charcoal

Practicals

Part 1: Potentiometry

a. Determination of solubility product of sparingly soluble silver salts.
b. Determination of dissociation constant of weak acids.
c. Potentiometric titrations:
    i) Redox titrations
        a) Fe^{2+}vs $Cr_2O_7^{2-}$
        b) Fe^{2+}vs Ce^{4+}
        c) I^-vs $KMnO_4$
    ii) Precipitation titration
        a) Cl^-vs Ag^+
        b) I^-vs Ag^+
        c) Mixture of Cl^- and I^-vs Ag^+

Part 2: Adsorption of oxalic acid/acetic acid on charcoal.

Part 3: Titration using pH meter – determination of dissociation constant of dibasic acid (Demonstration).

References:

1. W. J. Popiel, Laboratory Manual of Physical Chemistry, ELBS, London 1970
2. Findlay's Practical Physical Chemistry, B. P. Levitt, Longman, London, 1985
3. S. K. Sinha, Physical Chemistry A Laboratory Manual, Narosa Publishing Pvt, Ltd. 2014.

SEMESTER – III

Organic Synthesis

L (hrs)	Credit
60	4

Objectives

1. To understand about the pericyclic reactions
2. To learn about the rearrangements in photochemistry
3. To study about the reagents and rearrangements in Organic synthesis

Unit I Pericyclic Reactions-I (12 hrs.)

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems.

Unit II Pericyclic Reactions-II (12 hrs.)

Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Unit III Photochemistry (12 hrs.)

Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Bartons reaction and Photo-Fries rearrangement.

Unit IV Reagents in Organic Synthesis (12 hrs.)

Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

Unit V Rearrangements **(12 hrs.)**

General mechanistic considerations, nature of migration, migratory aptitude, nucleophilic, electrophilic and free radical rearrangement. A detailed study of various arrangements reactions.

References

1. Protective Groups in Organic Synthesis by T.W.Greene, Wiley-VCH, 1999.
2. Modern Heterocyclic Chemistry by L. A. Paquette, W.A. Benjamin, Inc.,1968.
3. Organic Chemistry by I. L. Finar, Vol II, ELBS,1968.
4. Heterocyclic Chemistry by T. R. Gilchrist, Longman,1989.
5. Selectivity in Organic Synthesis by Ward, Wiley-VCH,1999.
6. Robert E. Gawley, Jeffrey Aube, Principles of Asymmetric Synthesis, pergamon, 2nd edition, 1996
7. V.K. Ahluwalia and R.K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House, 2002.
8. J. March and M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 6th Edition, Wiley, 2007.
9. Fleming, Frontier Orbitals and Organic Chemical Reactions, Wiley, London, 1976.
10. S. Sankararaman, Pericyclic Reactions- A text Book, Wiley VCH, 2005

Electrochemistry

Objectives

L (hrs)	Credit
60	4

1. To study about the Interaction and Migrations of Ions.
2. To learn about the Electochemical measurement and Galvanic cells
3. To study about the Electrocatalysis, Photoelectrochemistry and Water splitting
4. To study about the Corrosion – types and its applications

Unit I Electrolytes & Electromechanical Interface (12 hrs.)

Ion-solvent interactions, ion-ion interactions, ionic migration and diffusion, Ionic activity, Debye-Huckel-theory, Electrolytic conductivity and the Debye-Hückel-Onsager Onsagar theory, Electrochemical interfaces – electrical double layer – Lippmann equation Helmholtz and Gouy – Chapman – Stern models of the double layer, Modern theories of electrical double layer. Adsorption of ions and dipoles.

Unit II Electrochemical Reaction & Equations (12 hrs.)

Galvanic cells: Reversible and Irreversible cells – EMF and its measurement, IUPAC convention for electrode potentials, Electrode potential Nernst equation, Electrochemical series, Activation, Ohmic and diffusion overpotentials, Activation polarisation, concentration polarisation, Current-potential relationship (derivation of Butler-Volmer and Tafel equations).

Unit III Electrochemical measurements (12 hrs.)

Electrochemical measurement: two electrode cell and three electrode cell, types of Reference Electrodes, working electrodes and counter electrodes, Current and diffusion controlled redox reactions, Reversible and Irreversible systems: Quasi-reversible systems, Steady-State Polarization Measurements, Transient (Pulse) Measurements, Impedance Measurements.

Unit IV Electrocatalysis & Photoelectrochemistry (12 hrs.)

Electrocatalysis: Introduction, Interaction of reactant with electrode, Mechanism and application of hydrogen and oxygen evolution reactions, Electrocatalyst for fuel cells.
Photoelectrochemistry: Principle of Photoelectrochemistry, charge–transfer process at Electrode/Electrolyte interface, photoelectrochemical cells and its Applications

(decontamination of water, water splitting, CO_2 Photoreduction).

Unit V Corrosion & Electrochemical sensors **(12 hrs.)**

Corrosion: Different types of corrosion; Pourbaix diagram, Stern Geary equation; mixed potential theory, corrosion rate measurements and prevention of corrosion.

Electrochemical sensors: Introduction to electrochemical sensors and biosensors, electrochemical sensors in environmental analysis, glucose biosensor, and immune sensors, ISFETs, CHEMFETS

References

1. Electrochemistry by Carl H. Hamann, Andrew Hamnett and WolfVielstich, Wiley VCH,2007.
2. Modern Electrochemistry 1. Volume 1 and 2, by J. O'M. Bockris and A. K.N. Reddy, Kluwer Academic, 2000.
3. Electrochemical Methods, by A. J. Bard and L. R. Faulkner, John Willey,2000, 2nd edition.
4. E. Gileadi, Physical Electrochemistry, Fundamental, Techniques and Applications, Wiley-VCH,2011
5. J. Bard and L. R Faulkner Electrochemical Methods: Fundamentals and Applications, 2nd Edition, Wiley,2001
6. P. H. Rieger, Electrochemistry, 2nd Edition, Springer1994
7. J. Newman and K. E. Thomas-Alyea, Electrochemical Systems, 3rd Edition, Wiley Interscience,2004
8. J. Wang, Analytical Electrochemistry, 3rd Edition, Wiley – VCH,2006
9. P.T.Kissinger and W.R. Heineman, Laboratory Techniques in Electroanalytical Chemistry, 2nd Edition, Marcel Dekker Inc.,1996

Bio-inorganic chemistry

L (hrs)	Credit
60	4

Objective

1. To study about the Role of alkaline and alkaline earth metal & Electron transfer.
2. To learn about the Oxygen transport and activation and Enzymes
3. To study about the Various spectroscopic methods in Bioinorganic chemistry
4. To study about the uses of Coordination complexes and Metals in medicine

Unit I Metals in Biology (12 hrs.)

Role of alkali and alkaline earth metal ions in biology; Na -K Pump, ionophores and crown ethers. Metal site structure, function. Metal ion transport and storage: Ferritin, Transferrin, Siderophores and metallothionein. Electron Transfer: Cytochromes, Iron-Sulfur Proteins and Copper Proteins.

Unit II Oxygen transport and activation and Enzymes (12 hrs.)

Oxygen transport and storage: Hemoglobin, myoglobin, hemerythrin, hemocyanin Oxygen activation: Cytochrome oxidase. Other metal containing enzymes: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, carbonic anhydrase, carboxypeptidase, vitamin B_{12} coenzyme, photosystem I and II, oxygen evolving center.

Unit II Spectroscopic methods in bioinorganic chemistry (12 hrs.)

Electronic spectra, EPR (emphasis on first row transition metal ions and their spectra), brief description of CD / MCD and multinuclear NMR. Applications of newer methods like EXAFS, XANES and ENDOR in characterization of biological molecules.

Unit IV Enzymes & Metabolism (12 hrs.)

Nitrogen-cycle enzymes : Mo in N, and S-metabolism by Mo-pterin cofactors and Mo- Fe-cofactors. NO_x reductases, sulfite oxidase, xanthine oxidase, nitrogenase, P and M-clusters in nitrogenase, transition-metal-dinitrogen complexes and insights into N_2 binding, reduction to ammonia.

Unit V Co-oordination complexes & Metals in Medicine (12 hrs.)

Use of coordination complexes as models for various enzymes, metalloproteins. Role of hazardous materials such as nitric oxide, cyanide and methyl isocyanate etc. in biological systems.

Metals in medicine - therapeutic applications of cis-platin, transition metal radio-isotopes (example: Tc, Co and Cu etc.) and MRI (Mn and Fe) agents. Toxicity of metals - Cd, Hg and Cr toxic effects with specific examples.

References:

1. S. J. Lippard and J. M. Berg, Principle of Bioinorganic Chemistry , University Science Books (1994).
2. Lawrence Que, Jr, Physical Methods in Bioinorganic Chemistry: Spectroscopy and Magnetism, University Science Books(2000).
3. F. A. Cotton and G. W. Wilkinson, Advanced Inorganic Chemistry, 5
John-Wiley & Sons, (1988). Page:8.
4. D. Banerjea, Coordination Chemistry, 2 Ed, Asian Books Pvt. Ltd. (2007).
5. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principal , Structure and Reactivity , 4 Ed. Harper Collins (1993). Page:7

Principles and Applications of Spectroscopy

Objective

L (hrs)	Credit
60	4

1. To study about the Vibrational and ESR spectroscopy
2. To learn about the NMR Spectroscopy
3. To know about the characterization of Mossbauer and UV- Visible spectroscopy
4. To study about the instrumentation of Mass spectroscopy

Unit I UV-Vis spectroscopy (12 hrs.)

Woodward rule for conjugated dienes and carbonyl compounds. IR: Characteristic vibrational frequencies of different functional groups, effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination and Fermi resonance bands

Unit II Vibrational & ESR spectroscopy (12 hrs.)

Vibrational: Symmetry and shapes of AB_2, AB_3, AB_4, AB_5 and AB_6, modes of bonding in ambidentate ligands, application of resonance Raman spectroscopy particularly for the study of active sites of metalloproteins.

Electron Spin Resonance: Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensor, application of transition metal complexes having one unpaired electrons.

Unit III Nuclear Magnetic Resonance (12 hrs.)

The contact and pseudo contact shifts, factors affecting nuclear relaxation, Chemical shift, spin-spin interaction, shielding mechanism. Shift reagent, spin tickling, nuclear overhauser effect (NOE), resonance of other nuclei. ^{13}C NMR: Chemical shift, ^{13}C coupling constants, two-dimensional NMR spectroscopy, NOISY, DEPT, INEPT terminology.

Unit IV Mossbauer spectroscopy (12 hrs.)

Principle, isomer shift, quadruple and magnetic interactions, information on oxidation state, π-back coordination, structure and nephelauxetic effect in iron compounds; Application to the studies of bonding and structures of Fe^{2+} and Fe^{3+} compounds including those of intermediate spin, studies on halides of tin(II) and tin(IV) compounds.

.

Unit V Mass spectroscopy (12 hrs.)

Instrumentation, Mass spectral fragmentation of organic compounds, Mc Lafferty rearrangement, examples of mass spectral fragmentation of organic compounds with respect to their structure determination.
ORD & CD: Definition, deduction of absolute configuration, octant rule for ketones.

References

1. Physical Methods in Chemistry by R. S. Drago, Saunders,1992
2. Inorganic Electronic Spectroscopy by A. B. P. Lever, Elsevier, 1984, 2ndEd.
3. Spectrometric Identifications of Organic Compounds by R. M.Silverstein, John Wiley,1991.
4. Introduction to Spectroscopy by D.L. Pavia, G. M. Lampman, G. S.Kriz, Harcourt College Publisher, NY,2001.
5. Organic Spectroscopy by William Kemp, ELBS 3rd Ed. 1994.

INORGANIC CHEMISTRY PRACTICAL- I

Objectives

P (hrs)	Credit
60	2

1. To train identification of metal ions in a mixture with semi micro qualitative analysis technique
2. To train the estimation of metal ions in a mixture by complexometric titration method

Practicals

a. Semi micro qualitative analysis of inorganic mixture containing two less-familiar cations.- W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U and Li.

b. Complexometric titrations – Estimation of Cu, Zn and Mg by EDTA titration in the presence of either Pb or Ba; estimation after elimination of Pb or Ba.

c. Determination of Total hardness, Ca and Mg content of water by EDTA titration.

References:

1. V.V. Ramanujam, 'Inorganic Semi micro Qualitative analysis, 3rd revised Edn, The National publishing Co., Chennai, 1988.
2. 'Vogel's Text Book of Quantitative Chemical Analysis', Eds. G.H. Jeffrey, J. Banett, J. Mendham and R.C. Denney, ELBS, 5thEdn. Reprint 1991.

INORGANIC CHEMISTRY PRACTICAL – II

Objective

P (hrs)	Credit
60	2

1. To provide training in separation and estimation of metal ions by volumetric and gravimetric methods of analysis

Practicals

Separation and estimation of metal ions in a mixture by volumetric and gravimetric methods. Some typical recommended mixtures are:

Cu(II) & Ni(II); Fe(II) & Cu(II); Cu(II) & Zn(II); Ca(II) & Ba(II); Fe(II) & Ni(II);
Cu(II) &Ca(II)

References:

1. 'Vogel's Text Book of Quantitative Chemical Analysis', Eds. G.H. Jeffrey, J. Banett, J. Mendham and R.C. Denney, ELBS, 5thEdn. Reprint 1991.

SEMESTER IV

Elective Papers

Supramolecular Chemistry

L (hrs)	Credit
45	3

Objectives

1. To study about the Ions Interactions
2. To learn about the Host Guest Interactions
3. To know about the Crystal Engineering and Molecular devices
4. To study about the recent developments in Supramolecular chemistry

Unit I Introduction of supramolecular chemistry (9 hrs.)

Definition of supramolecular chemistry. Nature of binding interactions in supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and vander Waals interactions.

Unit II Synthesis and structure of Macromolecules (9hrs.)

Synthesis and structure of crown ethers, lariat ethers, podands, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands and hemicarcerands., Host-Guest interactions, pre-organization and complimentarity, lock and key analogy.

Unit III Bonding reactions in supramolecular chemistry (9 hrs.)

Binding of cationic, anionic, ion pair and neutral guest molecules. Self-assembly molecules: design, synthesis and properties of the molecules, self assembling by H-bonding, metal-ligand interactions and other weak interactions, metallomacrocycles, catenanes, rotaxanes, helicates and knots.

Unit IV Crystal engineering & Molecular devices (9 hrs.)

Crystal engineering: role of H-bonding and other weak interactions

Molecular devices: molecular electronic devices, molecular wires, molecular rectifiers, molecular switches, molecular logic.

Unit V Advanced supramolecular chemistry (9 hrs.)

Relevance of supramolecular chemistry to mimic biological systems: cyclodextrins as enzyme mimics, ion channel mimics, supramolecular catalysis etc.

Examples of recent developments in supramolecular chemistry from current literature.

References

1. J.-M. Lehn; Supramolecular Chemistry-Concepts and Perspectives (Wiley-VCH, 1995)
2. P. D. Beer, P. A. Gale, D. K. Smith; Supramolecular Chemistry (Oxford University Press,1999)
3. J. W. Steed and J. L. Atwood; Supramolecular Chemistry (Wiley, 2000).
4. Desiraju, Raman Vittal, Crystal Engineering, University Press, 2019.
5. e-PG Pathshala- P-14- Organic Chemistry-IV (Supramolecular Chemistry).

Advanced Quantum Chemistry

L (hrs)	Credit
45	3

Objectives

1. To know about the introduction of Quantum chemistry
2. To learn about the Schrodinger equations and Wave functions
3. To know about the molecular and electronic structure of linear and non- linear molecule
4. To study about the PI Electron systems

Unit I Operator concept (9 hrs.)

Vector Interpretation of Wave function, Hermitian Operator, The Generalized Uncertainty principle, The quantum Mechanical Virial Theorem, Solution of harmonic oscillator (Operator approach), Second quantization (Boson and Fermion), Quantum theory of angular momentum, One electron Atom, Spin angular momentum.

Unit II Approximate solutions to the Schrodinger equation (9 hrs.)

The Variation method (Time independent and Time Dependent), Time independent perturbation theory (non – degenerate and degenetrate), Time dependent perturbation theory.

The Anti symmetry Principle, Spin angular momenta and their Operators, The Orbital Approximation (Slater- determinant, Pauli exclusion principle), Two electron wave functions.

Unit III The Hartree-Fock Self-Consistent Field Method (9 hrs.)

The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation energy, Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree-Fock Equations (Roothaan's equations).

Unit IV MO Methods (9 hrs.)

Introduction to Molecular Structure: The Born - Oppenheimer Approximation, Solution of the Nuclear Equation, Molecular Hartree- Fock Calculations.

Semiempirical Molecular Orbital Methods I - PI Electron Systems: The Huckel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method.

Semiempirical Molecular Orbital Methods II - All valence - Electron systems: The Extended Huckel Method, The CNDO Method.

Unit V Electronic Structure of Linear & Non-linear Molecule (9 hrs.)

Electronic Structure of Linear Molecule: The MO - LCAO Approximation, The Hydrogen Molecule Ion, H_{+2},The Hydrogen molecule, Molecular Configuration- Interactions, The Valence Bond Method, Molecular Perturbation Calculations.

Electronic Structure of Non-linear Molecule: The AH_n molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.

References:

1. Elementary Quantum Chemistry by Frank L. Pilar, 2nd Edition, McGraw -Hill Publishing Company,1990.
2. Molecular Quantum Mechanics by P. W. Atkins and R. S. Friedman, 3rd Edition, Oxford Univ. Press,1997.
3. Quantum Chemistry by D. A. Mc Quarrie, Oxford Univ. Press, 1983.
4. Quantum Chemistry by I. N. Levine, Allyn and Bacon Inc., 3rd Edition, May 1983.

Molecular Clusters

L (hrs)	Credit
45	3

Objectives

1. To know about the introduction of Molecular Clusters
2. To learn about the Transition Metal Clusters
3. To know about the Crystal Structure and Electrical Properties of Molecular clusters

Unit I Introduction of molecular clusters (9 hrs.)

Main-group clusters: Geometric and electronic structure, three-, four- and higher connect clusters, the closo-, nido-, arachno-borane structural paradigm, Wade- Mingos and Jemmis electron counting rules.

Unit II Metal - carbonyl clusters (9 hrs.)

Low nuclearity metal-carbonyl clusters and 14n+2 rule, high nuclearity metal-carbonyl clusters with internal atoms. Structure, synthesis and reactivity.

Unit III Transition-metal clusters (9 hrs.)

Main-group-Transition-metal clusters: Isolobal analogous of p-block and d-block clusters, limitations and exceptions.

Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters.

Unit IV Crystal Structure (9 hrs.)

Crystalline and amorphous solids; One and two dimensional lattices, crystal systems, Bravais lattices, point groups: α-Po, fcc, bcc and hcp metals and their packing efficiency, ionic radii ratios; Frenkel and Schottky defects, colour centers, Crystallographic shear (CS) in WO_3-x.

Unit V Electrical properties of clusters (9 hrs.)

Band theory of solids -metals and their properties; semiconductors - extrinsic and intrinsic, Hall effect; thermoelectric effects (Thomson, Peltier and Seebeck); insulators - dielectric, ferroelectric, pyroelectric and piezoelectric properties, multiferroics.

References

1. D. M. P. Mingos and D. J. Wales; Introduction to Cluster Chemistry, Prentice Hall, 1990.
2. N. N. Greenwood and E. A. Earnshaw; Chemistry of elements, Second Edition, Butterworth- Heinemann,1997.
3. T. P. Fehlner, J. F. Halet and J-Y. Saillard; Molecular Clusters: A Bridge to solid- state Chemistry, Cambridge University press,2007.
4. B. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, Universities Press (India),2010.
5. D. M. P. Mingos, Essential Trends in Inorganic Chemistry, Oxford, University Press,1998.
6. C. E. Housecroft, Metal-Metal Bonded Carbonyl Dimers and Clusters, Oxford Chemistry Primers (44), Oxford, University Press,1996.
7. R. West, Solid State Chemistry and its Applications, John Wiley &Sons, 1984, 2nd edition, 2014.
8. L. E. Smart and E. A. Moore, Solid State Chemistry - An Introduction, 4th Edition, CRC Press,2012.
9. H. V. Keer, Principles of the Solid State, 2nd Edition, New Age International, 2017.
10. M. Weller, T. Overton, J. Rourke and F. Armstrong, Inorganic Chemistry, 6th Edition, Oxford University Press, 2014. (South Asia Edition2015).
11. e-PG Pathshala- P-11- Inorganic Chemistry-III (Metal Clusters)

Polymer Chemistry

L (hrs)	Credit
45	**3**

Objectives

1. To know about the Concept of Macro molecules
2. To learn about the Polymerization process and Polymer stereochemistry
3. To know about the Industrial and Conducting Polymers

Unit I Concept of macromolecules (9 hrs.)

Principle of duality – molecular design – nomenclature and classification – raw material sources of polymers – classification of polymers - synthetic schemes – Molecular Weight determination.

Unit II Polymerization processes (10hrs.)

Free radical and addition polymerization; kinetics and mechanism, Chain transfer – molecular weight distribution and molecular weight control; Radical atom transfer and fragmentation – addition mechanism, Free radical living polymers, cationic and anionic polymerization- kinetics and mechanism.

Unit III Polymer Stereochemistry (10hrs.)

Stereoregularity in polymers – isotactic, syndiotactic and atactic polymers; polar and non-polar polymers; stereospecific polymerization and the utility of Ziegler-Natta catalyst; Copolymerization – bulk solution, melt, suspension, emulsion and dispersion techniques; synthesis of graft and block copolymers.

Unit IV Organic polymers & Industrial polymers (8 hrs.)

Semiconducting properties of organic polymers containing metal groups – semiconduction of biopolymers and its application to biochemical problems – superconductors.

Industrial polymers – Synthesis, Structure and applications of industrially important polymers.

Unit V Conducting polymers (8hrs.)

Synthesis of conducting polymers - chemical structure and electronic behavior of polymers – doping of conducting polymers – p- & n- type doping – doping techniques;

References

1. F. W. Billmeyer, Textbook of polymer Science, 3rdEdn, Wiley, New York, 1991.
2. V. R. Gowariker, N. V. Viswanathan, J. Sreedhar, Polmer Science, Wiley-Eastern, New Delhi, 1988.
3. Tager, Physical Chemistry of Polymers, Mir Publishers, Moscow, 1978.
4. R. J. Young, Principles of Polymer Science, 3rdEdn., Chapman and Hall, New York, 1991.
5. P. J. Flory, Polymer Science, Cornell University Press, Ithacka, 1953.
6. J. E. Katon, Organic Semiconducting Polymers, Marcel Dekker, New York, 1968.
7. Bahadur, N. V. Sastry, Principles of Polymer Science, Narosa, New Delhi, 2002.
8. e-PG Pathshala – P-06- Physical Chemistry –II (M-31-Polymers and their Classification)

Nuclear Chemistry

L (hrs)	Credit
45	3

Objectives

1. To know about the Radiactivity
2. To learn about the Nuclear reactions and Nuclear reactor
3. To know about the Applications of Radioactivity

Unit I Radioactivity and its Measurement (9 hrs.)

Discovery – types of decay – decay kinetics – half-life period, mean life, parent-daughter decay – growth relationship – secular and transient equilibrium; Units of radioactivity; alpha, beta and gamma decay; Theory of decay, energies and properties.

Unit II Nuclear Reactions (9 hrs.)

Artificial radioactivity. Detectors: ionization chamber, electron pulse counter, scintillation detectors. Nuclear fission, fusion, photonuclear reactions and thermonuclear reactions.

Unit III Nuclear Reactor (9 hrs.)

The fission energy – reproduction factor; Classification of reactors based on moderators, coolants, phase of fuel and generation. Breeder reactor India's nuclear energy programmes – reprocessing of spent fuels.

Unit IV Radiation and Matter (9 hrs.)

Application of radioisotopes: probing by isotopes, reactions involved in the preparation of radioisotopes. The Szilard-Chalmers' reaction – Radiochemical principles in the use of Tracers

Unit V Applications of Radioactivity (9 hrs.)

Applications of radioisotopes as tracers – chemical investigations, analytical applications, agricultural and industrial applications – Neutron activation analysis – Carbon and rock dating .

References

1. S. Glasstone, Source book on atomic energy, East West press, 3rdEdn,2014.
2. H.J. Arniker, Essentials of Nuclear Chemistry, New Age International, Reprint 2011.

3. M.G. Friedlander, J.M. Kennedy, E.S. Macian and J.M. Miller, Nuclear and Radiochemistry, 3rd Edn. John Wiley & Sons, 1981.
4. M.G. Arora and M. Singh, Nuclear Chemistry, Anmol Publications, 2002.

Pharmaceutical Chemistry

Objectives

L (hrs)	Credit
45	3

1. To know about the Mechanism of drug action
2. To learn about the Synthesis of drugs
3. To know about the Enzymes and Nucleic acids

Unit I Mechanism of drug action (9 hrs.)

Introduction to the history of pharmaceutical chemistry, general mechanisms of drug action on lipids, carbohydrates, proteins and nucleic acids, drug metabolism and inactivation, receptor structure and sites, drug discovery development, design and delivery systems, gene therapy and drug resistance.

Unit II Synthesis of drugs (10 hrs.)

Classification of drugs based on structure and pharmacological basis with examples. Synthesis of important drugs such as α-methyl dopa, Chloramphenicol, griseo fulving, cephelosphorins and nystatin. Molecular modeling, conformational analysis, qualitative and quantitative structure activity relationships.

Unit III Action of antibiotics (10hrs.)

General introduction to antibiotics, mechanism of action of lactam antibiotics and anon lactam antibiotics, antiviral agents, chemistry, stereochemistry, biosynthesis and degradation of penicillins – An account of semisynthetic pencillins – acid resistant, pencillinase resistant and broad spectrum semisynthetic pencillins.

Unit IV Enzymes (8hrs.)

Elucidation of enzyme structure and mechanism, kinetic, spectroscopic, isotopic and stereochemical studies. Chemical models and mimics for enzymes. Design, synthesis and evaluation of enzyme inhibitors.

Unit V Nucleic acids (8 hrs.)

DNA-protein interaction and DNA-drug interaction. Introduction to rational approach to drug design, physical and chemical factors associated with biological activities, mechanism of drug action.

References

1. A. Kar, Medicinal Chemistry, New Age International (P) Ltd, Delhi, 1997.
2. Principles of Biochemistry - L. Stryer (W.H. Freeman & Co.), 2002.
3. Principles of Biochemistry - A.L.Lehninger, D.W.Nelson & M.M.Cox (Macmillan), 1991.
4. Biochemistry - D.Voet & J.G.Voet (John Willey), 1995.
5. Harper's Illustrated Biochemistry - R.K.Murray et al. (McGraw Hill), January 8, 2005.
6. Lehninger's Principle of Biochemistry by David L. Nelson and Michael M. Cox. W. H. Freeman; 4th edition (2004).
7. Text Book of Biochemistry with clinical correlation by Thomas .M. Devlin, John Wiley-Liss, Hobokhen NJ publishers (2006).
8. A text book of pharmaceutical chemistry, Jayashree ghosh, S. Chand, 2003.
9. Medicinal chemistry, G.R.Chatwal, Himalaya Publishing House, New Delhi (2002)
10. Pharmacology and Pharmatherapeutics – R.S. Satoskar and S.D. Bhandarkar, 1973.

Elective II- Photochemistry & Surface Chemistry(e- learning course)

Objectives

L (hrs)	Credit
45	**3**

1. To know about the Photochemical reactions
2. To learn about the Synthesis, Properties and charge transfer of Ruthenium Complexes
3. To know about the Surface Catalysis and Adsorption Isotherm

Unit I Photochemistry – I (9 hrs.)

Properties of excited states, electronically excited states of metal complexes and charge transfer excitations - bimolecular deactivation and energy transfer processes; ligand field photochemistry – photosubstitution, photoisomerisation and photoredox reactions;

Unit II Photochemistry – II (9 hrs.)

Synthesis, properties and charge transfer photochemistry of $[Ru(bpy)_3]^{2+}$ - photochemical conversion and storage of solar energy - photochemistry at semiconductor electrodes –Honda cell and water photolysis.

Unit III Surface chemistry – I (9 hrs.)

Gibbs adsorption isotherm – surface films – spreading of one liquid on another – measurement of film pressure; solid-liquid interfaces – contact angle – wetting as a contact angle phenomenon – wetting as a capillary action phenomenon.

Unit Surface chemistry-II (9 hrs.)

Physisorption , chemisorptions –Langmuir, Freundlich and BET isotherms - surface area determination – heats of adsorption; heterogeneous catalysis – role of surfaces in catalysis – semiconductor catalysis – n-and p-type surfaces.

Unit V Kinetics of surface (9 hrs.)

Reactions involving adsorbed species – Langmuir- Hinshelwood mechanism – Langmuir – Rideal mechanism. Detergency – general aspects of soil removal – factors in detergent action; foams and aerosols.

References:

1. J.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, Wiley Eastern Revised Edn, 1978.
2. J. Chem. Ed., October 1983 issue, American Chemical Society
3. A.W. Anderson and F.D. Fleischer, Concepts of Inorganic Photochemistry, John Wiley and Sons, New York, 1975.
4. A.W. Adamson, Physical Chemistry of Surfaces, 5th Edition, John Wiley and Sons, New York, 1990.
5. S. Glasstone, Text Book of Physical Chemistry, 2nd Edition, Macmillan India Ltd, New Delhi , 1974.
6. K.J. Laidler, Chemical Kinetics, 2nd Edition, Tata McGraw –Hill, New Delhi 1991.
7. J.C. Kuriacose, Catalysis, Macmillan India Ltd., New Delhi, 1991.
8. e-PG Pathshala- P-14- Organic Chemistry-IV (Surface Chemistry).

Advanced Organic practical

P (hrs)	Credit
60	2

Objectives

1. To study about the various types of separation methods for organic compounds
2. To study about the various distillation methods for organic compounds
3. To study about the various characterization methods for organic compounds

Practicals

a. Distillation Methods: Fractional distillation, Azeotropic Distillation, Distillation under reduced pressure and Steam distillation.
b. Separation of organic compounds: Paper chromatography, TLC and Column chromatography.
c. Characterization of organic compounds: UV, FT-IR, Gas chromatography (GC), and LCMS.

References

1. R.M. Silverstein, G.C. Bassler, T.C. Morril, Spectrometric Identification of Organic Compounds, John Wiley & Sons, New York, 1991.
2. W. Kemp, Organic Spectroscopy, Macmillan Press Ltd. 1996.
3. Jag Mohan, Organic Spectroscopy, Principles and Applications, Narosa publishing House, New Delhi, 2001.
4. P.R.Young, Practical Spectroscopy, The Rapid Interpretation of Spectral Data Brooks/Cole, California, 2000.
5. R. Davis, M. Frearson, Mass Spectrometry, John Wiley & Sons, New York, 1991.

Advanced Inorganic practical

Objectives

P(hrs)	Credit
60	**2**

To provide skills in preparation and characterization of metal complexes

Practicals

1. Analysis and characterization of metal complexes by UV VIS & IR spectral, other physico-chemical techniques. Some typical analysis is:
   a. Determination of Δ_o of by UV VIS spectroscopy
   b. Confirmation of metal-ligand bond & complex formation by IR spectroscopy
2. Preparation and characterization of Inorganic nanomaterials (Metal and Metal oxide) by XRD, SEM-EDX, UV-VIS, IR.
3. Water quality analysis by Laboratory methods.
4. Evaluate and report the corrosion parameters for given metal samples in various electrolytes.

References:

1. G. Pass & H. Sutcliffe, Practical Inorganic Chemistry, Science paperbacks, Chapman and Hall, London, 1974.
2. R. Gopalan& V. Ramalingam, Concise Coordination Chemistry, Vikas Publishing House Pvt. Ltd., NewDelhi 2000.
3. R.S. Drago, Physical Methods in Chemistry, W.B. Saunders, 1997. 4. E.A. V. Ebsworth et al., Structural Methods in Inorganic Chemistry, ELBS 1987.
4. Nanomaterials: Synthesis, Characterization, and Applications, 1st Edition, A. K. Haghi, Ajesh K. Zachariah, Nandakumar Kalarikkal, Apple Academic Press 2013
5. An introduction to nanoparticles and nanotechnology, Maria Benelmekki, Book chapter, Morgan & Claypool Publishers 2015.
6. Handbook of Methods in Environmental Studies VOL.l Water and Wastewater Analysis, S.K.Maiti, ABD Publisher 2005.
7. Mars G. Fontana, Corrosion Engineering, Mc Graw Hill series in Materials Science and Engineering,1987.

Advanced Physical practical

P (hrs)	Credit
60	2

Objectives

To provide training in analysis of chemical compounds using some instrumental techniques

Practicals

Part 1: Spectrophotometry

a. Mixture analysis - Determination of concentration of two components in a given mixture ($KMnO_4$& $K_2Cr_2O_7$).

b. Determination of metal ions (lead, calcium, magnesium) from water samples using calibration curve method.

Part 2: Electrochemical analysis

a. Determination of redox potentials of organic and inorganic molecules.

b. Amperometric titration of $Pb(NO_3)_2$ with $K_2Cr_2O_7$.

Part 3: Surface analysis

a. Surface area analysis and pore size measurement using BET surface analyzer from porous materials.

Part 4: pHmetry

a. Determination of dissociation constants of tribasic acid (phosphoric acid).

b. Determination of some physical parameters of water samples (eg.: alkalinity).

References:

1. A. Findary, T. A. Kitchner, Practical physical chemistry. (Longmans, Green and Co.), 1935.
2. J. M. Wilson, K. J. Newcombe, A. R. Denko, R. M. W. Richett, Experiments in Physical Chemistry, (Pergamon Press), 1963.
3. D. P. Shoemaker, C. W. Garland, Experiments in Physical Chemistry, McGraw-Hill. New York, 1967.