VISVESVARAYA TECHNOLOGICAL UNIVERSITY, BELAGAVI.

Syllabus

M.Sc. in Chemistry

(Specialisation: Forensics / Nano **/** Pharmaceutical Chemistry**)**

(Effective from the Academic year 2023-24)

I SEMESTER

CONCEPTS OF ORGANIC CHEMISTRY			
Course Code	22MSC11	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Stereoisomerism: Projection formulae [flywedge, Fischer, Newman and sawhorse], enantiomers, diastereoisomers, mesomers, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS configurational notations.

Optical isomerism: Conditions for optical isomerism: Elements of symmetry-plane of symmetry, centre of symmetry, alternating axis of symmetry (rotation-reflection symmetry). Optical isomerism due to chiral centers and molecular dissymmetry, allenes and biphenyls, criteria for optical purity.

Module-2

Geometrical isomerism: Due to C=C, C=N and N=N bonds, *E*, *Z* conventions, determination of configuration by physical and chemical methods. Geometrical isomerism in cyclic systems.

Conformational analysis: Elementary account of conformational equilibria of ethane, butane and cyclohexane. Conformation of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanones and decalins.

Conformational analysis of 1,2-, 1,3- and 1,4- disubstituted cyclohexane derivatives and *D*-Glucose, Effect of conformation on the course and rate of reactions.

Stereoselectivity: Meaning and examples of stereospecific reactions, stereoselective reactions, diastereoselective reactions, regioselective, regiospecific reactions, enantioselective reactions and enantiospecific reactions.

Module-3

Basics of organic reactions: Meaning and importance of reaction mechanism, classification and examples for each class.

Bonding in organic systems: Theories of bonding-molecular orbital approaches. Huckel molecular orbital theory and its application to simple π-systems: ethylene, allyl, cyclopropyl, butadienyl, cyclopentadienyl, pentadienyl, hexatrienyl, cyclohexatrienyl,

heptatrienyl, cycloheptatrienyl systems. Calculation of the total π-energy, and M.O. coefficients of the systems.

Aromaticity: Concept of aromaticity, Huckel's rule, Polygon rule, annulenes, heteroannulenes and polycyclic systems.

Structure and reactivity: Brief discussion on effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases.

Module-4

Methods of determining organic reaction mechanism: Thermodynamic and kinetic requirements for reactions, kinetic and thermodynamic control. Identification of products. Determination of reaction intermediates, isotope labeling and effects of cross over experiments. Kinetic and stereochemical evidence, solvent effect. Formation, structure, stability, detection and reactions of carbocations (classical and non-classical), carbanions, free radicals, carbenes, nitrenes, arynes and ylides (Sulphur, nitrogen and phosphorous).

Aliphatic Nuleophilic Substitution reactions: Kinetics, mechanism and

stereochemical factor affecting the rate of S_N^1, S_N^2, S_{RN}^i, S_N^i, $S_N^{1'}$, $S_N^{2'}$, S_N^{1i} and S_{RN}^1 reactions,

Neighbouring group participation.

Electrophilic substitution reactions: Kinetics, mechanism and stereochemical factor

affecting the rate of S_E^1 & S_E^2

Module-5

Aromatic electrophilic substitution reactions: Mechanism of nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier Haack reaction, Diazonium coupling, Gattermann–Koch reaction, Mercuration reaction.

Aromatic nucleophilic substitution reactions: S_N^1, S_N^2 and benzyne mechanism, Bucherer reaction, von Richter reaction.

Mechanism of Addition reactions: Addition to C=C multiple bonds involving electrophiles, nucleophiles. Markownikoff's rule and anti-Markownikoff's rule.

Additions to carbonyl compounds: Addition of water, alcohol, bisulphate, HCN and amino compounds. Hydrolysis of esters.

Elimination reactions: Mechanism and stereochemistry of eliminations - E_1, E_2, $E_{1c}B$. *cis* elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution reactions, decarboxylation reactions. Chugaev reaction.

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. Minimum passing marks in SEE is 40% of the maximum marks of SEE. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each subject/ course if the student secures not less than 50% (50 marks out of 100) in the sum total of the CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) taken together.

Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. Stereochemistry of carbon compounds, Ernest L. Eliel.
2. Stereochemistry: P. S. Kalsi.
3. Organic Chemistry, VI edition, Robert T. Morrison, Robert N. Boyd.
4. Organic Chemistry, Vol-I by I. L. Finar.
5. Advance Organic Chemistry, IV edition, Jerry March.
6. Advance Organic Chemistry, III edition, Part-A and Part-B, Francis A. Carey and Rechard J. Sundberg.
7. Organic Chemistry, III edition, V. K. Ahluwalia and Rakesh Kumar Parashar.
8. Reactive intermediates in Organic Chemistry, N. S. Isaacs.

CONCEPTS OF INORGANIC CHEMISTRY			
Course Code	22MSC12	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Chemical Periodicity: Review of periodic properties

Structures and energetics of ionic crystals: Introduction, MX (NaCl, CsCl, ZnS) and MX2 (fluorite, rutile, β-crystobalite, cadmium chloride and cadmium iodide) types. The perovskite and spinel structures. Thermodynamics of ionic crystal formation. Hydration energy and solubility of ionic compounds, Lattice energy, Born-Haber cycle, Born-Lande equation.The Kapustinskii's equation, Consequences of lattice enthalpies.Applications of lattice energetics. Ionic radii, factors affecting the ionic radii, radius ratio rules.

Module-2

Structures and energetics of inorganic molecules: Introduction, Bent's rule, Energetics of hybridization. VSEPR model for explaining structure of moleculesincluding fluxional molecule. M.O. treatment of homo-nuclear and heteronuclear diatomic molecules. M.O. treatment involving delocalized π-bonding (CO_3^{2-}, NO_3^-, NO_2^-, CO_2 and N_3^-), M.O. correlation diagrams (Walsh) for triatomic molecules.

Modern concept of acids and bases: Lux-Flood and Usanovich concepts, solvent system and leveling effect. Hard-Soft Acids and Bases, Classification and Theoretical backgrounds.

Module-3

Non-aqueous solvents: Classification of solvents, Properties of solvents (dielectric constant, donor and acceptor properties) protic solvents (anhydrous H2SO4, HF and glacial acetic acid) aprotic solvents (liquid SO_2, BrF_3 and N_2O_4). Solutions of metals in liquid ammonia, hydrated electron. Super acids and super bases. Heterogeneous acid base reactions.

Ionic liquids: Molten salt solvent systems, Ionic liquids at ambient temperature, Reactions in and applications of molten salt/ionic liquid media.

Supercritical fluids: Properties of supercritical fluids and their uses as solvents. Supercritical fluids as media for inorganic chemistry

Module-4

Lanthanoid chemistry: General trends, Electronic, optical and magnetic properties. Abundance and extraction, **General principles**: conventional, solvent extraction and ion-exchange methods. Separation from monazite. Chemistry of principal oxidation states (II, III and IV). Stability of tetrahalides, dihalides and aqua ions of simple lanthanide compounds. Redox potentials.**Uses:** lanthanides as shift reagents, lanthanides as probes in biological systems. High temperature super conductors.

Module-5

Actinoid chemistry: General trends and electronic spectra**.** Occurrence and preparation of elements, **Isolation of the elements**: thorium and uranium, enrichment of uranium for nuclear fuel, uranium hydrides, oxides and chlorides. Chemical reactivity and trend. Chemistry of trans-uranium elements.

Supramolecular Chemistry: Introduction, selectivity and Supramolecular Interactions.

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Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. Basic Inorganic Chemistry – 3rd edition. F.A. Cotton, G. Wilkinson and P.L. Gaus, John Wiley and Sons (2002).
2. Inorganic Chemistry, 3rd edition. James E. Huheey, Harper and Row Publishers (1983).
3. Inorganic Chemistry, 5th edition. G.L. Miessler, P. J. Fischer and D.A. Tarr, Pearson (2014).
4. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
5. Inorganic Chemistry, 4th edition. C.E. Housecroft and A.G. Sharpe, Pearson Education Ltd. (2012).
6. Introduction to Modern Inorganic Chemistry, K.M. Mackay and R.A. Mackay, Blackie Publication (1989).
7. Concepts and Models of Inorganic Chemistry 3rd edition. B.E. Douglas, D.H. McDaniel and Alexander, Wiley (2001).
8. Ionic liquids-Classes and Properties (Ed) by Scott T. Handy, Intech Publisher (2011).
9. Lanthanide and Actinide Chemistry, Simon Cotton, John Wiley and Sons Ltd., (2006).
10. Supramolecular Chemistry, Peter J. Cragg, Springer (2010).

KINETICS, PHOTOCHEMISTRY AND CATALYSIS			
Course Code	22MSC13	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Chemical Kinetics: Complex reactions: Kinetics of parallel, consecutive and reversible reactions. Chain reactions: Branched chain reactions, general rate expression, Auto catalytic reactions (Hydrogen-Oxygen reaction), oscillatory reactions and explosion limits.

Theories of reaction rates: Collision theory and its limitations, Activated complex theory (postulates - derivation) and its applications to reactions in solution. Energy of activation, other activation parameters - determinations and their significance. Lindemann theory, Hinshelwood's theory of unimolecular reactions.

Module-2

Potential energy surfaces: Features and construction, theoretical calculations of Ea.

Reactions in solution: Ionic reactions - salt effects, effect of dielectric constant (single and double sphere models). Effect of pressure, volume and entropy change on the rates of reactions. Cage effect with an example.

Fast reactions- Introduction, study of fast reactions by continuous and stopped flow techniques, relaxation methods (T-jump and P-jump methods), flash photolysis, pulse and shock tube methods.

Module-3

Photochemistry: Introduction to photochemistry, laws of photochemistry, laws of light absorption, quantum yield and its determination, factors affecting quantum yield, Actinometry - Uranyloxalate and potassium ferrioxalate actinometers, acetone and diethylketone actinometers. Term symbols for atoms and its significance.

Photochemical properties of electronically excited molecules, nature of changes on electronic excitation, shapes of absorption band and Frank Condon principle. Experimental techniques to determine the intermediates in photochemical reactions. Photosensitization: by mercury, dissociation of H2. Photochemical kinetics of: Decomposition of CH3CHO, formation of HI and HCl. Fluorescence and phosphorescence – theory and applications. Resonance fluorescence and quenching of fluorescence,
Kinetics of colliosional quenching (Stern-Volmer equation).

Module-4

Homogeneous Catalysis: Electronic and structural effects on acidity and basicity. Hard and soft acids and bases. Acidity functions: Hammet acidity function, Zucker-Hammet hypothesis, Bonnett hypothesis. Industrial catalysis: Catalyst carrier, promoter, inhibitor and catalyst poison.

Enzyme kinetics: Effect of substrate concentration (Michaelis - Menton equation), Effect of pH, effect of catalysts and inhibitors (substrate, zeolite, Cr3+, Fe2+ ZnO, U.V light), effect of temperature. A brief kinetic and mechanistic applications of glucose oxidase in the oxidation of glucose.

Module-5

Linear Free Energy Relationship: Hammett equation, Taft equation, Okemoto Brown equation and its application to oxidation of amino acids and aromatic amines. Swain- Scott and Edward equation. Winstein - Grunwald relationship. Isokinetic relationship and significance of isokinetic temperature, Exner criterion.

Kinetic Isotope Effect: Theory of kinetic isotope effect - normal and inverse isotope
effect, primary isotope effect, secondary isotope effect, solvent isotope effect.

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Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks**

to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).
2. Elements of Physical Chemistry by Lewis and Glasstone, 2nd Edn. Macmillan & Co Ltd., New York.
3. Chemical Kinetics by K.J. Laidler, Tata McGraw-Hill Pub, Co Ltd, New Delhi.
4. Chemical Kinetics by Frost and Pearson.
5. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose, Macmillan, New Delhi.
6. Chemical Kinetics by L.K. Jain.
7. Photochemistry, Calvert and Pitts, Wiley, New York (1996).
8. Fundamentals of Photochemistry, Gohatgi-Mukherjee, New Age International Ltd., 1986.
9. Principles and Applications of Photochemistry, R. P. Wayne, Elsevier, New York (1970).
10. Photochemistry, Paul Suppan, RSC, London (1994).
11. Chemical Kinetics by K.J. Laidler, Tata McGraw-Hill Pub, Co Ltd, New Delhi.
12. Fundamentals of Chemical Kinetics, M. R. Wright, Harwood publishing, Chichesrer, 1999.
13. Kinetics and Mechanism of Chemical Transformation by J. Rajaram and J.C. Kuriacose, Macmillan, New Delhi.

PRINCIPLES OF QUANTUM MECHANICS			
Course Code	22MSC14	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:0	SEE Marks	50
Total Hours of Pedagogy	30	Total Marks	100
Credits	2	Exam Hours	3

Module-1

Quantum Chemistry: Introduction to quantum mechanics: Schrödinger wave equation, time-independent and time dependent Schrödinger wave equation and the relation between their solutions. Eigen functions and Eigen values. Physical interpretation of wave function. Concept of operators – Laplacian, Hamiltonian, Linear and Hermitian operators. Angular momentum operators and their properties. Commutative and noncommutative operators..

Module-2

Normalization, orthogonality and orthonormality of wave functions. Postulates of quantum mechanics. Solutions of Schrödinger wave equation for free particles, particle in a ring, particle in three dimensional box. Quantum mechanical degeneracy, tunnelling (no derivation). Wave equation for H-atom separation and solution of R, ϕ and θ equations. Application of Schrodinger equation to rigid rotator and harmonic oscillator. Eigen functions and Eigen values of angular momentum. Ladder operator method for angular momentum.

Module-3

Variation theorem: Statement and proof, application of variation theorem to a particle in one dimensional box, linear oscillator, H and He-atoms. **Approximation methods:** Time Independent Perturbation Theory - Degenerate and Non-generate case.

Module-4

Molecular orbital theory, LCAO-MO approximation, application to hydrogen molecule ion (H_2^+), energy levels of H_2^+, bonding and antibonding molecular orbitals, energy distribution, potential energy diagrams. Valence bond theory (VB), theory of H_2 molecule, Heitler-London method, energy levels, various modifications of Heitler-London wave function. Comparison of MO and VB theories. SCF method for many electron atom.

Module-5

Slater Orbitals –Effective nuclear charge (ENC), expressions for slater orbitals for 1s, 2s, 3s, 2p and 3d electrons (no derivation), Slater's rules for calculation of ENC. Theories of valence – Introduction, linear and non-linear variation functions, secular equations, coulombic, exchange, normalization and overlap integrals,secular determinants.

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Semester-End Examination:

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- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. Introductory Quantum Chemistry – A.K. Chandra. Second Edition, Tata McGraw Hill Publishing Co. Ltd., (1983).
2. Quantum Chemistry – Eyring, Walter and Kimball. John Wiley and Sons, Inc., New York.
3. Quantum Chemistry –I.N. Levine. Pearson Education, New Delhi, (2000).
4. Theoretical Chemistry – S. Glasstone. East West Press, New Delhi, (1973).
5. Quantum Chemistry – R.K. Prasad, New Age International Publishers, (1996).
6. Valence Theory – Tedder, Murel and Kettle.

SOLID STATE CHEMISTRY			
Course Code	22MSC15	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:0	SEE Marks	50
Total Hours of Pedagogy	30	Total Marks	100
Credits	2	Exam Hours	3

Module-1

Crystal morphology: symmetry elements, crystal systems; Bravais lattices; Crystal planes and directions: Miller indices, interplanar separations. Crystal symmetry, Symmetry elements and symmetry operations. Structure analysis by X-rays: Atomic scattering factor; Laue conditions for diffraction and Bragg's law; Geometrical structure factor, systematic absences; Powder X-ray diffraction.

Module-2

Packing in a crystal: BCC, FCC, HCP structures with examples. Point defects, line defects, plane defects. Free electron theory of metals, Band theory of solids, Effective mass; Direct and Indirect bandgaps: Determination of bandgap; Donors and acceptors, carrier concentration at thermal equilibrium; Calculation of Fermi level; Degenerate and Nondegenerate semiconductors.MO band and zone theories.

Module-3

Imperfections in atomic packing: Types of imperfections, classification of imperfections, point defects, Schottky defects, Frenkel defects, disordered crystals, line defects, dislocation types, plane defects, small-angle and large-angle boundaries, stacking faults, crystal growth and twinning, non-stoichiometry.
Imperfections and physical properties: electrical, optical, magnetic, thermal and mechanical properties

Module-4

Semiconducors - intrinsic and extrinsic, Hall Effect, Insulators-dielectric, ferroelectric, pyroelectric and Peizoelectric properties, Magnetic properties-Dia, para, ferro, ferri, antiferro and antiferri materials, Defects and dislocations-Vacancies and interstitials, dislocations and grain boundaries colour centers and reactivity, Amorphous materials-glasses and refractories, Superconductivity-Theory and its application.

Module-5

Diamagnetism and Paramagnetism: Langevin's diamagnetism equation, Quantum theory of diamagnetism of mononuclear systems, Quantum theory of paramagnetism, Hund's rule, Paramagnetic susceptibility of conduction electrons, Ferro, Anti and Ferri magnetism: Curie point and the exchange integral, Magnons, Ferrimagnetic order, Curie temperature and susceptibility of ferrimagnets, Antiferromagnetic order. Weiss theory of ferromagnetism, Ferromagnetic domains, Bloch walls, Origin of domains, Novel magnetic materials: GMRCMR materials.

Assessment Details (both CIE and SEE)

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Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**
CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. D.A McQuarrie and J.D. Simon, Physical Chemistry, a molecular approach, University Science Books.
2. Tareen and Kutty, Solid state chemistry.
3. Lesley Smart & Elaine Moore, SolidState Chemistry, nelson Thornes.
4. A.K. Galway, Chemistry of Solids, Science Paperbacks and Chapman and Hall Ltd., London 91967).
5. A.R. West, basic Solid State Chemsitry, John Wiley & Sons Ltd. (1991).
6. B.S.Skoog and D.M. West, Principles of Instrumental Analysis, Sanndes College, Philadelphia (1980).
7. Atomic structure and chemical Bond, Manas Chanta **Publisher:** McGraw-Hill Inc.,US (1 December 1974) **ISBN-10:** 0070965110
8. Concise Inorganic chemistry, J.D.Lee **Publisher:** Wiley; 5th edition edition (18 December 1998) **ISBN-10:** 0632052937
9. Inorganic Chemistry, G. Wwfsberg Unit IV **Publisher:** Pearson; 4 edition (31 May 2012) **ISBN-10:** 0273742752
10. Introduction to solids – L.V. Azaroff **Publisher:** McGraw Hill Education; New edition edition (14 June 2001) **ISBN-10:** 0070992193
11. Introduction to solid state Physics – C. Kittel **Publisher:** John Wiley & Sons Inc (23 July 1996) **ISBN-10:** 0471142867
12. Elements of solids state physics, J.P. Srivastava **Publisher:** Prentice Hall India Learning Private Limited; 4th Revised edition edition (17 December 2014) **ISBN- 10:** 8120350669
13. Superconductivity and Superconducting Materials – A V Narlikar and S N Ekbote (South Asian Pub., 1983).
14. Physics of high Tc superconductors – J C Phillips (Academic Press, 1989)
15. Introduction to superconductivity – A C Rose-Innes and E H Rhoderick (Pergamon Press, 1978)

RESEARCH METHODOLOGY AND IPR			
Course Code	22MSC16	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:0	SEE Marks	50
Total Hours of Pedagogy	30	Total Marks	100
Credits	2	Exam Hours	3

M.Tech. common paper syllabus

INORGANIC CHEMISTRY PRACTICALS			
Course Code	22MSC17	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	0:6:0	SEE Marks	50
Total Hours of Pedagogy	72	Total Marks	100
Credits	3	Exam Hours	3

PART – A

1. Determination of iron in haematite using cerium (IV) solution (0.02M) as the titrant, and gravimetric estimation of insoluble residue.
2. Estimation of calcium and magnesium carbonates in dolomite using EDTA titration, and gravimetric analysis of insoluble residue.
3. Determination of manganese dioxide in pyrolusite using permanganate titration.
4. Quantitative analysis of copper-nickel in alloy/mixture:
    i. Copper volumetrically using KIO3.
    ii. Nickel gravimetrically using DMG
5. Determination of lead and tin in a mixture: Analysis of solder using EDTA titration.
6. Quantitative analysis of chloride and iodide in a mixture:
    i. Iodide volumetrically using KIO_3
    ii. Total halide gravimetrically
7. Gravimetric analysis of molybdenum with 8-hydroxyquinoline.
8. Quantitative analysis of copper(II) and iron(II) in a mixture:
    i. Copper gravimetrically as CuSCN and
    ii. Iron volumetrically using cerium(IV) solution
9. Spectrophotometric determinations of:
    i. Titanium using hydrogen peroxide
    ii. Chromium using diphenyl carbazide in industrial effluents
    iii. Iron using thiocyanate/1,10-phenanthroline method in commercial samples
    iv. Nickel using dimethylglyoxime in steel solution
10. Micro-titrimetric estimation of :
    i. Iron using cerium(IV)
    ii. Calcium and magnesium using EDTA
11. Quantitative estimation of copper (II), calcium (II) and chloride in a mixture.

PART – B

Semimicro qualitative analysis of inorganic mixtures containing **TWO** anions and **TWO** cations (excluding sodium, potassium and ammonium cations) and **ONE** of the following less common cations: W, Mo, Ce, Ti, Zr, V and Li.

Assessment Details (both CIE and SEE)

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Continuous Internal Evaluation (CIE):

CIE marks for the practical course is **50 Marks**.

The split-up of CIE marks for record/ journal and test are in the ratio **60:40**.

- Each experiment to be evaluated for conduction with observation sheet and record write-up. Rubrics for the evaluation of the journal/write-up for hardware/software experiments designed by the faculty who is handling the laboratory session and is made known to students at the beginning of the practical session.
- Record should contain all the specified experiments in the syllabus and each experiment write-up will be evaluated for 10 marks.
- Total marks scored by the students are scaled downed to 30 marks (60% of maximum marks).
- Weightage to be given for neatness and submission of record/write-up on time.
- Department shall conduct 02 tests for 100 marks, the first test shall be conducted after the 8th week of the semester and the second test shall be conducted after the 14th week of the semester.
- In each test, test write-up, conduction of experiment, acceptable result, and procedural knowledge will carry a weightage of 60% and the rest 40% for viva-voce.
- The suitable rubrics can be designed to evaluate each student's performance and learning ability.
- The average of 02 tests is scaled down to **20 marks** (40% of the maximum marks).

The Sum of **scaled-down** marks scored in the report write-up/journal and average marks of two tests is the total CIE marks scored by the student.

References

1. Vogel's Text Book of Quantitative Chemical Analysis – 5th edition, J. Basset, R.C. Denney, G.H. Jeffery and J. Mendhom.
2. A Text Book of Quantitative Inorganic Analysis by A.I. Vogel, 3rd edition.
3. Spectrophotometric Determination of Elements by Z. Marczenko.
4. Vogel's Qualitative Inorganic Analysis – Svelha.
5. Macro and SemimicroInorganicQualitative Analysis by A.I. Vogel.
6. Semimicro Qualitative Analysis by F.J. Welcher and R.B. Halin.
7. 7. Quantitative Chemical Analysis by Daniel C. Harris, 7th edition, (2006).

II SEMESTER

MECHANISM OF ORGANIC REACTIONS			
Course Code	22MSC21	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Concepts, Types of Rearrangements, Rearrangement to electron deficient carbon: (carbon migration) Wagner-Meerwin rearrangement, Pinacol-Pinacolone rearrangement.

Rearrangement to electron rich carbon: Stevens rearrangement, Sommelet-Hauser rearrangement, Wittig rearrangement. Rearrangement to electron deficient nitrogen: Hofmann rearrangement, Curtius rearrangement, Schmidt rearrangement, Beckmann rearrangement. Rearrangement to electron deficient oxygen: Baeyer Villiger reaction, Hydroperoxide rearrangement, Dakin reaction. Intra-molecular migration from nitrogen to carbon: Jacobsen rearrangement**.** Intermolecular migration from nitrogen to carbon:

Aromatic arrangements: Orton rearrangement, Fischer-Hepp rearrangement, Hofmann-Martius rearrangement, Bamberger Rearrangement, Migratory aptitude in rearrangements, cross-over experiments and its significance.

Module-2

Castro-Stephens coupling, Baylis Hillman reaction, Eschenmoser methenylation, Evans Aldolreaction, Staudinger reaction, Horner-Wadsworth-Emmons reaction, McMurry coupling, Nazarov cyclization, Nef reaction, Ritter reaction and Pauson-Khand reaction.

Eschenmoser-Tanabe Fragmentation, Hofmann-Loffler-Freytag reaction, Julia-Lythogoe olefination, Koenig-Knorr glycosidation, Mitsunobu reaction, Mukaiyama aldol reaction, Peterson olefination, Hayashi reaction, Shapiro reaction, Sharpless asymmetric epoxidation, Sommelet reaction, Von Braun reaction, Hofmann-Loffler Freytag reaction,

Ramburg-Backland reaction. Hell- Volhard- Zelinski reaction. Haloform reaction. Claisen ester condensation, Darzen reaction, Dieckmann, Perkin and Prins reactions. Mannich reaction. Michael reaction, Robinson anulation. Wittig reaction.

Module-3

General principles, Photosensitization and PET reactions, Photochemistry of carbonyl compounds. Photochemistry of alkenes, Photochemistry of aromatic compounds, Norrish Type I and II, Patterno Buchi reaction, Barton reactions, chemi and bioluminescence reactions, Photochemical rearrangements- aromatic rearrangements, Dienone rearrangements, Di-pimethane rearrangements, Photo-Fries rearrangements. Definition and types of reactions classified as pericyclic actions - (a) Cycloaddition and cycloconversion

(b) Electrocyclic ring closing and ring opening (c) Sigmatropicre-arrangements (d) Cheletropic reactions (e) Group transfers,

Module-4

Stereochemistry of pericyclicreactions and theory of molecular orbital symmetry. Application of theory of M.O.Symmetry by the method of correlation diagram by both thermal and photochemical paths. Stereochemistry of Pericyclic reactions-thermal and photochemical by "Method of transition state atomaticity".

Basic principles of perturbation molecular orbital (PMO)theory, significance of Frontier Molecular orbitals, Stereochemistry of pericyclic reactions by the "Frontier molecular orbital (FMO) method".

Module-5

Elements of a synthesis (Reaction methods, reagents, catalysts, solvents, protecting groups (Hydroxyl, Amino Carbonyl and Carboxylic acid protecting groups), activating groups, leaving groups, synthones and

synthetic equivalents. Types of selectivities (Chemo, Regio and Stereo selectivity). Synthetic Planning illustrated by simple molecules, disconnections and functional group inter conversions. Umpolung reactions and use in synthesis. Retro synthetic analysis of a complex molecule-a case study.

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. Minimum passing marks in SEE is 40% of the maximum marks of SEE. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each subject/ course if the student secures not less than 50% (50 marks out of 100) in the sum total of the CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) taken together.

Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. J. March, Advanced Organic Chemistry. 4th Edition, Wiley Interscience New York.
2. R.O.C. Norman and E.M. Coxon, Principles in Organic Synthesis, 2005, CRC Press, New York.
3. Jie Jack Li – Name Reactions: A Collection of Detailed Reaction Mechanisms. Laszlo Kurti and Barbara Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.
4. J. Singh, Photochemistry and Pericyclic Reactions, New Age International, 2005.
5. John McMurry, Organic Chemistry, 5 Ed., 2000 or newer.
6. Stuart Warren, Designing organic synthesis: programmed introduction to the synthon approach, 1994.
7. Carruthers, Modern Synthetic Methods, Cambridge

CHEMICAL THERMODYNAMICS			
Course Code	22MSC22	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Chemical Thermodynamics: Entropy: Physical significance, entropy changes in an ideal gas. Variation of entropy with temperature, pressure and volume. Entropy changes in reversible and irreversible processes.

Free energy: Helmholtz and Gibbs free energies, Gibbs-Helmholtz equation and its applications, Maxwell's relations and its applications. Nernst heat theorem: its consequences and applications. Third law of thermodynamics: statements, applications and comparison with Nernst heat theorem.

Module-2

Partial molar properties: Physical significance, determination of partial molar volumes by intercept method and from density measurements. Chemical potential and its significance. Variation of chemical potential with temperature and pressure. Formulation of the Gibbs – Duhem equation. Derivation of Duhem-Margules equation.

Fugacity: Relation between fugacity and pressure, variation of fugacity with temperature and pressure. Determination of fugacity of gases.

Activity and activity coefficient: Variation of activity with temperature and pressure. Determination of activity co-efficient by vapour pressure, depression in freezing point, solubility measurements and by electrical methods.

Thermodynamics of dilute solutions: Raoult's law, Henry's law. Ideal and non-ideal solutions.

Module-3

Non-equilibrium thermodynamics. Thermodynamics of irreversible processes. Stationary state. Principle of local equilibrium. Forces and fluxes. The phenomenological relations. Onsagar relations. Coupled flows. Direct and Cross coefficients. Domination of direct coefficients Linear relations-proof. Reciprocal relation (no derivation).– Entropy production in simple irreversible system (closed systems). Application of reciprocal relation to irreversible processes. Thermal diffusion. Thermo-osmosis and thermo-molecular pressure difference. Electro kinetic phenomena. Entropy production in the process. Electro osmosis, streaming potential, streaming current and electro-osmotic pressure.

Module-4

Statistical thermodynamics: Objectives of statistical thermodynamics, concept of distribution, types of ensembles. Thermodynamic probability and most probable distribution law. Partition functions – definition, evaluation of translational, rotational and vibrational and electronic partition functions for monoatomic, diatomic and polyatomic gaseous molecules. Sackur-Tetrode equation for entropy of translation function. Calculation of thermodynamic functions and equilibrium constants in terms of partition functions. Different distribution laws (Types of statistics): Maxwell- Boltzmann, Bose-Einstein and Fermi-Dirac Statistics (derivation of the three distribution laws). Comparison of Bose-Einstein and Fermi-Dirac Statistics with Maxwell-Boltzmann statistics. Problems and their solutions.

Module-5

Phase rule studies: Thermodynamic derivation of phase rule. Application of phase rule to the two component systems - compound formation with congruent melting point and incongruent melting points, Roozeboom's classification. Application of phase rule to three component systems- systems of three liquids and systems of two salts and water.

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. Minimum passing marks in SEE is 40% of the maximum marks of SEE. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each subject/ course if the student secures not less than 50% (50 marks out of 100) in the sum total of the CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) taken together.

Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. I Prigogine, An introduction to the Thermodynamics of Irreversible processes. Inrterscience.
2. Allen J. Bard and Larry Faulkner, Electrochemical methods : Fundamentals and applications, Wiley
3. Gurdeepraj, Advanced Physical Chemistry, Goel Publishing
4. L K Nash, Elements of Statistical Thermodynamics, Addison Wesley Publishing Co.
5. G K Vemulapalli, Physical Chemistry, Prentice-Hall of India.
6. Text Book of Physical Chemistry by Samuel Glasstone, MacMillan Indian Ltd., 2nd edition (1974).

ELECTROCHEMISTRY			
Course Code	22MSC23	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Electrochemistry of solutions: Factor effecting electrolytic conductance. Debye- Huckel theory - Concept of ionic atmosphere. Debye-Huckel-Onsager equation of conductivity and its validity. Debye-Huckel limiting law (DHL), its modification for appreciable concentrations. A brief survey of Helmholtz-Perrin, Guoy-Chapman and Stern electrical double layer (no derivation). Transference number: True and apparent transference numbers, Abnormal transference numbers, effect of temperature on transference numbers. Liquid junction potential-determination and minimization.

Module-2

Energetics of cell reactions: Effect of temperature, pressure and concentration on energetics of cell reactions (calculation of ΔG, ΔH and ΔS). Electrical Double layer: Theories of Double-Layer structure, diffuse-double-layer theory of Gouy and Chapman, the Stern Model, Adsorption of ions and neutral compounds, Electrocaplillary and differential capacitance measurements; Influence of double layer on charge transfer processes.

Module-3

Irreversible electrode process: Introduction, reversible and irreversible electrodes, reversible and irreversible cells. Polarization, over voltage - concentration over voltage, activation over voltage and ohmic over voltage. Experimental determination of over voltage. Equations for concentration over potential, stationary and non-stationary surface. Butler-Volmer equation, Tafel equation. Hydrogen oxygen over voltage. Effect of temperature, current density and *p*H on over voltage. Polarography- Half wave potential, application in qualitative and quantitative analysis.

Module-4

General principles of Potentiometry, different types of electrodes. Principle of chronopotentiometry. Voltammetry, Different potential types. Linear sweep, differential pulse and cyclic voltammetry. Polarography- principle. Micro electrode, potential and current variations at the micro electrode systems. Applications of polarography. Principles and applications of Amperometry, Coulometry and anodic stripping voltammetry.

Module-5

Surface confined electrochemical processes: The fundamentals of corrosion. Homogeneous and heterogeneous electrocatalysis (HER and OER). Electrochemical processes coupled to chemical steps. Nanostructured and surface modified electrodes. Introduction to batteries, fuel cells and electrochemical solar cells. Electrochemical processes of particular relevance to energy conversion

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. Minimum passing marks in SEE is 40% of the maximum marks of SEE. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each subject/ course if the student secures not less than 50% (50 marks out of 100) in the sum total of the CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) taken together.

Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks**

to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. D. I. Antropov, Theoretical Electrochemistry, Mir Publishers, 1972.
2. J. M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol.1 and 2, Plenum Press, 1998.
3. Industrial Electrochemistry, 2nd ed, Pletcher, Derek/Walsh, Frank C., London: Chapman and Hall, 1990
4. Electrochemistry for Chemists, 2nd ed, Sawyer, Donald T./Sobkowiak, Andrej/Roberts, Julian L., New York: John Wiley, 1995
5. Introduction to Electrochemistry by S. Glasstone, Affiliated East-West Press, New Delhi,
6. Electrochemistry –Principles and Applications by E.G. Potter, Cleaver-Hume press Ltd, London.
7. Modern Electrochemistry Vol. I and II by J.O.M. Bockris and A.K.N. Reddy, Pentium Press, New York (1970).

INTRODUCTION TO NANOSCIENCE			
Course Code	22MSC24	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:0	SEE Marks	50
Total Hours of Pedagogy	30	Total Marks	100
Credits	2	Exam Hours	3

Module-1

Feynmann's vision on nanoscience & technology, bulk vs nanomaterials, natural and synthetic nanomaterials. Quantum confinement in nanostructures- size dependent physical phenomena in semiconductor and metal nanoparticles. Classification of nanostructures, 0D, 1D and 2D nanostructures. Visualization of nanostructures and techniques related.

Module-2

Surface energy and surface stress-origin and estimation of surface energy. Surface Energy minimization:- Sintering Ostwald ripening and agglomeration. Energy minimization by Isotropic and anisotropic surfaces. Surface energy and surface curvature, Surface energy stabilization- electrostatic stabilization, steric stabilization, electro-steric stabilization..

Module-3

Kinetics of phase transformations, Homogeneous & Heterogeneous nucleation. Controlling nucleation, growth and aggregation in nanoparticle growth. Growth Mechanisms: Spontaneous growth, Evaporation condensation growth, growth controlled by diffusion and surface process, VLS growth, fundamentals of thin film growth.

Module-4

Diamond – Graphite- Fullerenes, CNTs and Graphene. Synthesis: CVD, Laser and Electrochemical and other methods. Functionalization and reactivity of CNTs.

Module-5

Micro & Mesoporous Materials, Ordered mesoporous structures, Random mesoporous structures, and crystalline microporous materials: zeolites. Core – Shell Structures – Metaloxide structures, Metal-polymer structures, Oxide-polymer structures. Organic-Inorganic Hybrids- Class I hybrids, Class II hybrids, Intercalation Compounds.

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. Minimum passing marks in SEE is 40% of the maximum marks of SEE. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each subject/ course if the student secures not less than 50% (50 marks out of 100) in the sum total of the CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) taken together.

Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. Nanostructures and Nanomaterials- Synthesis, Properties & applications by Guozhong Cao, Imperial College Press, (2006). (for UNIT I & II, 2nd Chapter, Unit III Chapter 4 (3.2), Unit IV- Chapter 7
2. Nanomaterials and Nanochemistry by C. Brechignac.P. Houdy M. Lahmani Springer- Verlag (2007). (For Unit III-Part I Chapter I)
3. Materials Science and Engineering-An Introduction 7e, William D. Callister, (Wiley, 2007). (Chapter 10. section 1-.2 and 10.3) Unit II.
4. Introduction to Nanoscience & Nanotechnology by Gabor L. Hornyak, Harry F. Tibbals, Joydeep Dutta, John J. Moore, CRC Press, Tylor & Francis Group New York, 2009. **Publisher:** CRC Press (15 December 2008) **ISBN-13:** 978-1420047790
5. Introduction to Nanoscale Science & Technology, Di Ventra, Evoy, Heflin, Springer Science, NY, 2004. **Publisher:** Springer; 1 edition (30 June 2004) **Sold by:** Amazon Asia-Pacific Holdings Private Limited.

MOLECULAR SPECTROSCOPY			
Course Code	22MSC25	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	2:0:0	SEE Marks	50
Total Hours of Pedagogy	30	Total Marks	100
Credits	2	Exam Hours	3

Module-1

Microwave spectroscopy: Rotation spectra of diatomic Molecules - rigid and non rigid rotator model. Rotational quantum number and the selection rule. Effect of isotopic substitution on rotation spectra. Classification of polyatomic molecules based on moment of inertia. Rotation spectra of polyatomic molecules (OCS CH3F and BCl3).

Moment of inertia expression for linear tri-atomic molecules. Applications – Principles of determination of Bond length and moment of inertia from rotational spectra. Stark effect in rotation spectra and determination of dipole moments.

Module-2

Vibration spectroscopy*:* Vibration of diatomic molecules, vibrational energy curves for simple harmonic oscillator. Effects of anharmonic oscillation, expressions for fundamental and overtone frequencies. Vibration - rotation spectra of carbon monoxide.

Vibration of polyatomic molecules – The number of degrees of freedom of vibration. Parallel and perpendicular vibrations (CO2 and H2O). Combination, difference and hot bands. Fermi resonance. Force constant and its significance. Theory of infrared absorption and theoretical group frequency. Intensity of absorption band and types of absorptions. Applications: Structures of small molecules: XY2 – linear or bent, XY3 – planar or pyramidal

Module-3

Raman spectroscopy: Introduction, Raman and Rayleigh scattering, Stokes and anti- Stokes lines, polarization of Raman lines, depolarization factor, polarizability ellipsoid.

Theories of Raman spectra - classical and quantum theory. Rotation-Raman and vibration-Raman spectra. Raman activity of vibrations, rule of mutual exclusion principle. Vibration modes of some simple molecules and their activity.

Resonance Raman Spectroscopy: Resonance Raman Effect and its applications. Nonlinear Raman effects: Hyper, stimulated and inverse Raman effects. Coherent Anti- Stokes Raman Scattering and its applications.

Module-4

UV Visible spectroscopy: Quantitative aspects of absorption – Beer's law, Technology associated with absorption measurements. Limitations– real, chemical, instrumental and personal. Theory of molecular absorption. Vibration- rotation fine structure of electronic spectra. Types of absorption bands- n to π*, π to π*, n to σ* and σ to σ*, C-T and ligand field. Instrumentation.

Module-5

Applications: Qualitative and quantitative analysis of binary mixtures, measurements of dissociation constants of acids and bases, determination of molecular weight. Woodwards empirical rules for predicting the wavelength of maximum absorption for olefins, conjugated dienes, cyclic trienes and polyenes, α,ß-unsaturated aldehydes and ketones, benzene and substituted benzene rings.

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. Minimum passing marks in SEE is 40% of the maximum marks of SEE. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each subject/ course if the student secures not less than 50% (50 marks out of 100) in the sum total of the CIE (Continuous

Internal Evaluation) and SEE (Semester End Examination) taken together.

Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. Fundamentals of Molecular Spectroscopy, C.N. Banwell and E.M. McCash. 4th edition, Tata McGraw Hill, New Delhi.
2. Fundamentals of molecular spectroscopy, G. M. Barrow, MgGraw Hill, New York (International students Edition), 1974.
3. Theoretical chemistry, S. Glasstone, affiliated East-West Press Pvt. Ltd, New Delhi, 1973.
4. Spectroscopy, B.P. Straughan and S. Walker, John Wiley & Sons Inc., New York Vol. 1 and 2, 1976.
5. Vibration Spectroscopy Theory and Applications, D.N. Satyanarayana, New Age International, New Delhi (2004).
6. Spectroscopy, B.P. Straughan and S. Salker, John Wiley and Sons Inc., New York, Vol.2, 1976.
7. Organic Spectroscopy, William Kemp, English Language Book society, Macmillan, 1987.
8. Instrumental methods of analysis, H. H. Willard, L. L. Merritt and J. A. Dean, 7th Edition, 1988.
9. Physical methods in inorganic chemistry, R. S. Drago, affiliated East-West press Pvt. Ltd., (Student Edition) 1978.

PHYSICAL CHEMISTRY PRACTICALS			
Course Code	22MSC27	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	0:6:0	SEE Marks	50
Total Hours of Pedagogy	72	Total Marks	100
Credits	3	Exam Hours	3

PART - A

1. Study of kinetics of hydrolysis of methyl acetate in presence of two different concentrations of HCl/H2SO4 and report the relative catalytic strength.
2. Study of kinetics of reaction between K2S2O8 and KI, first order, determination of rate constants at two different temperatures and *E*a.
3. To study the kinetics of saponification of ethyl acetate by conductivity method at two different concentrations of NaOH and report the relative catalytic strength.
4. Determination of partial molar volume of salt-water system (NaCl-H_2O/KCl-H_2O/KNO_3-H2O) systems.
5. To study the kinetics of reaction between acetone and iodine - determination of order of reaction with respect to iodine and acetone.
6. Study the kinetics of decomposition of diacetone alcohol by NaOH, determine the catalytic coefficient of the reaction and comparison of strength of alkali.
7. Determination of energy of activation for the bromide-bromate reaction.
8. Kinetics of reaction between sodium formate and iodine and determination of energy of activation.
9. Determination of heat of solution of organic acid (benzoic acid/salicylic acid) by variable temperature method (graphical method).
10. Determination of degree of association of benzoic acid in benzene by distribution method.
11. To determine the eutectic point of a two component system (Naphthalene-*m*dinitrobenzene system).
12. Analysis of a binary mixture (Gylcerol & Water) by measurement of refractive index.
13. Determination of the molecular weight of a polymer material by viscosity measurements (cellulose acetate/methyl acrylate).

PART - B

1. Conductometric titration of a mixture of HCl and CH_3COOH against NaOH.
2. Conductometric titration of sodium sulphate against barium chloride.
3. pH titration of (a) HCl against NaOH (b) Copper sulphate against NaOH and (c) CH_3COOH/HCOOH against NaOH - determination of Ka.
4. Determination of equivalent conductance of weak electrolyte (CH_3COOH) at infinite dilution following Kohlrausch law.
5. Determination of dissociation constant and mean ionic activity coefficient of weak acids (CH_3COOH/HCOOH/$ClCH_2COOH$) by conductivity method.
6. Potentiometric titration of KI *vs* KMnO4 solution.
7. Determination of dissociation constant of a weak acid (CH_3COOH/HCOOH/$ClCH_2COOH$) by potentiometric method.
8. Potentiometric titration of a mixture of halides (KCl+KI/KCl+KBr/KBr+KI) against $AgNO_3$.
9. To obtain the absorption spectra of coloured complexes, verification of Beer's law and estimation of metal ions in solution using a spectrophotometer.
10. Potentiometric titration of $K_2Cr_2O_7$ against FAS determination of redox potential and concentration of Fe^{2+} ions.
11. Conductometric titration of oxalic acid against NaOH and NH_4OH.
12. Coulometric titration I_2 vs $Na_2S_2O_3$.

13. Determination of acidic and basic dissociation constant and isoelectric point of an amino acid by pH metric method.
14. Kinetics of photodegradation of indigocarmine (IC) using ZnO/TiO_2 as photocatalyst and study the effect of [ZnO/TiO_2] and [IC] on the rate of photodegradation.

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each course. The student has to secure not less than 40% of maximum marks in the semester-end examination(SEE). In total of CIE and SEE student has to secure 50% maximum marks of the course.

Continuous Internal Evaluation (CIE):

CIE marks for the practical course is **50 Marks**.

The split-up of CIE marks for record/ journal and test are in the ratio **60:40**.

- Each experiment to be evaluated for conduction with observation sheet and record write-up. Rubrics for the evaluation of the journal/write-up for hardware/software experiments designed by the faculty who is handling the laboratory session and is made known to students at the beginning of the practical session.
- Record should contain all the specified experiments in the syllabus and each experiment write-up will be evaluated for 10 marks.
- Total marks scored by the students are scaled downed to 30 marks (60% of maximum marks).
- Weightage to be given for neatness and submission of record/write-up on time.
- Department shall conduct 02 tests for 100 marks, the first test shall be conducted after the 8th week of the semester and the second test shall be conducted after the 14th week of the semester.
- In each test, test write-up, conduction of experiment, acceptable result, and procedural knowledge will carry a weightage of 60% and the rest 40% for viva-voce.
- The suitable rubrics can be designed to evaluate each student's performance and learning ability.
- The average of 02 tests is scaled down to **20 marks** (40% of the maximum marks).

The Sum of **scaled-down** marks scored in the report write-up/journal and average marks of two tests is the total CIE marks scored by the student.

References

1. Practical Physical Chemistry – A.J. Findlay.
2. Experimental Physical Chemistry – F. Daniels *et al*.
3. Selected Experiments in Physical Chemistry – Latham.
4. Experiments in Physical Chemistry – James and Prichard.
5. Experiments in Physical Chemistry – Shoemaker.
6. Advanced Physico-Chemical Experiments – J. Rose.
7. Practical Physical Chemistry – S.R. Palit.
8. Experiments in Physical Chemistry – Yadav, Geol Publishing House.
9. Experiments in Physical Chemistry – Palmer.

10. Experiments in Chemistry – D.V. Jahagirdar, Himalaya Publishing House, Bombay, (1994).
11. Experimental Physical Chemistry – R.C. Das and B. Behera, Tata Mc Graw Hill.

III SEMESTER

ADVANCED ORGANIC CHEMISTRY			
Course Code	22MSC31	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Oxidation: Metal based and non-metal based oxidations of alcohols (chromium, manganese, silver, ruthenium, DMSO, and hypervalent iodine). (b) Peracids oxidation of alkenes and carbonyls. (c) Alkenes to diols (manganese, osmium based), alkenes to carbonyls with bond cleavage (manganese, ruthenium, and lead based, ozonolysis), and alkenes to alcohols/carbonyls without bond cleavage (hydroboration-oxidation, Wacker oxidation, and selenium based allylic oxidation).
(d) Asymmetric epoxidations (Sharpless, Jacobsen, and Shi epoxidations) and Sharpless asymmetric dihydroxylation.

Module-2

Reduction: (a) Catalytic homogeneous and heterogeneous hydrogenation, Wilkinson catalyst. (b) Metal based reductions using Li/Na in liquid ammonia, sodium, magnesium, zinc, titanium, and samarium. (c) Hydride transfer reagents: NaBH4, L- selectride, K-selectride, Luche reduction, LiAlH4, DIBAL-H, Red-Al, Trialkylsilanes, and Trialkylstannane. (d) Enantioselective reductions (Chiral Boranes, Corey-Bakshi-Shibata) and Noyori asymmetric hydrogenation.

Module-3

Modern Synthetic Methods: (a) Baylis-Hillman reaction, Henry reaction, Kulinkovich reaction, Ritter reaction, Sakurai reaction, Brook rearrangement, Tebbe olefination.
(b) Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed ortho metalation. (c) Stereoselective synthesis of tri- and tetra-substituted olefins, Synthetic applications of Claisen rearrangement, ene reaction (metallo-ene, Conia ene).

Module-4

Construction of Ring Systems: (a) Different approaches towards the synthesis of three, four, five, and six-membered rings. (b) Pauson-Khand reaction, Bergman cyclization; Nazarov cyclization, cation-olefin cyclization and radical-olefin cyclization, inter-conversion of ring systems (contraction and expansion). (c) Construction of macrocyclic rings and ring closing metathesis.

Module-5

Retrosynthetic Analysis: Basic principles and terminology of retrosynthesis, synthesis of aromatic compounds, one group and two group C-X disconnections, one group C-C and two group C-C disconnections, amine and alkene synthesis, important strategies of retrosynthesis, functional group transposition, important functional group interconversions Protecting groups: Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

Assessment Details (both CIE and SEE)

The weightage of Continuous Internal Evaluation (CIE) is 50% and for Semester End Exam (SEE) is 50%. The minimum passing mark for the CIE is 50% of the maximum marks. Minimum passing marks in SEE is 40% of the maximum marks of SEE. A student shall be deemed to have satisfied the academic requirements and earned the credits allotted to each subject/ course if the student secures not less than 50% (50 marks out of 100) in the sum total of the CIE (Continuous Internal Evaluation) and SEE (Semester End Examination) taken together.

Continuous Internal Evaluation:

- Three Unit Tests each of **20 Marks**
- Two assignments each of **20 Marks** or **one Skill Development Activity of 40 marks** to attain the COs and POs

The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

CIE methods /question paper is designed to attain the different levels of Bloom's taxonomy as per the outcome defined for the course.

Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from each module.
- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.

2. L. Kuerti and B. Czako, Strategic Applications of named Reactions in Organic Synthesis, Elsevier Academic Press, 2005.

3. J. Clayden, N. Greeves, S. Warren and P. Wothers, Organic Chemistry, Oxford University Press, 2001.

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6. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004.

7. J. Tsuji, Palladium Reagents and Catalysts, New Perspectives for the 21st Century, John Wiley & Sons, 2003.

8. I. Ojima, Catalytic Asymmetric Synthesis, 2nd edition, Wiley−VCH, New York, 2000.

9. R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley & Sons, 1994.

ADVANCED ANALYTICAL TECHNIQUES			
Course Code	22MSC32	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Microscopic Techniques: Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM). Scanning Probe Microscopy: Atomic Force Microscopy, Scanning Tunnelling Microscopy (STM), Near field scanning optical microscopy (NSOM). Principles of Fluorescence microscopy. Confocal Laser Scanning Microscopy.

Module-2

Techniques for Thermal & Mechanical Analysis: Thermal Analysis: TGA, DTG, DTA, DSC - combustion calorimetry- Thermal diffusivity by the laser flash technique- simultaneous techniques including analysis for gaseous products.

Mechanical testing- Introduction, tension testing, High strain rate testing of materials, Fracture Toughness testing methods, Hardness testing.

Module-3

Magnetic & Electrochemical Techniques: Magnetic Vibrating Sample Magnetometer, Mossbauer spectroscopy, ESR, NMR.

Magneto-optic Kerr effect. Electrochemical Techniques:Cyclic voltammetry, Electrochemical Impedance, Scanning electrochemical Microscopy, The quartz crystal micro balance.

Module-4

Structure and Surface Analysis Techniques: X-ray powder diffraction: principles and practices. Small angle X-ray diffraction, GIXRD, and Single crystalline X-ray diffraction. Hydrophobic and hydrophilic surfaces, Super hydrophobicity and hydrophilicity, Contact angle, BET surface area and porosity analysis.

Module-5

Electro-analytical technique Principle and applications of : Coulometry, Polarography, Hydrodynamic voltametry , Pulse Polarography , Cyclic Voltammetry and Amperometry,

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The sum of three tests, two assignments/skill Development Activities, will be **scaled down to 50 marks**

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Semester-End Examination:

- The SEE question paper will be set for 100 marks and the marks scored will be proportionately reduced to 50.
- The question paper will have ten full questions carrying equal marks.
- Each full question is for 20 marks. There will be two full questions (with a maximum of four sub-questions) from

each module.

- Each full question will have a sub-question covering all the topics under a module.
- The students will have to answer five full questions, selecting one full question from each module

References

1. Introduction to Nanoscience and Nanotechnology, by K K Chattopadhyay, PHI Learning Pvt. Ltd. New Delhi 2019, **ISBN-13:** 978-81-203-3608-7.
2. Characterization of Materials Vol 1 &2, by Elton N. Kaufmann, John Wiley and Sons Publication, 2003. New Jersey.
3. Principles of instrumental analysis, Douglas A Skoog, Donald M West, Saunders College, Philadelphia. **Publisher:** Cengage; 6 edition (1 November 2014) **ISBN- 13:** 978-81-315-25579.
4. NANO: The Essentials- Understanding Nanoscience and Nanotechnology, by T Pradeep, Tata McGraw Hill Education Pvt. Ltd. New Delhi)**ISBN-13:** 978-0-07- 061788-9
5. X-Ray Diffraction Procedures: For Polycrystalline and Amorphous Materials, 2nd Edition - Harold P. Klug, Leroy E. Alexander,**Publisher:** Wiley-Blackwell; 2nd Revised edition edition (1 January 1974) **ISBN-13:** 978-0471493693
6. Transmission Electron Microscopy: A Textbook for Materials Science (4-Vol Set)**-** David B. Williams and C. Barry Carter, **Publisher:** Springer; 1st ed. 1996. Corr.6thprinting edition (15 April 2005) **ISBN-13:** 978-0306453243
7. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM **-** Ray F. Egerton ,**Publisher:** Springer; Softcover reprint of hardcover 1st ed. 2005 edition (12 October 2010) **ISBN-13:** 978-1441938374
8. Springer handbook of Nanotechnology ed. Bharat Bhushan (Springer), **Publisher:** Springer-Verlag (15 May 2006) **ISBN-13:** 978-3540343660.

ADVANCED INORGANIC TECHNIQUES			
Course Code	22MSC33	CIE Marks	50
Teaching Hours/Week (L:P:SDA)	3:0:2	SEE Marks	50
Total Hours of Pedagogy	50	Total Marks	100
Credits	4	Exam Hours	3

Module-1

Fundamental concepts: Introduction, Classification of organometallic compounds by bond type, nomenclature, the effective atomic number rule, complexes that disobey the EAN rule, common reactions used in complex formation.

Organometallics of transition metals: Preparation, bonding and structures of nickel, cobalt, iron and manganese carbonyls. Preparation and structures of metal nitrosyls.

Ferrocene: Preparation, structure and bonding**. Metal-carbene and metal-carbyne complexes**.

Complexes containing alkene, alkyne, arene and allyl ligands: Preparation, structure and bonding

Module-2

General principles of Catalysis: Language of catalysis. Homogeneous and heterogeneous catalysts.

Homogeneous catalysis - Industrial Applications: Alkene hydrogenation and hydroformylation, The Wacker's process, Monsanto acetic acid process and L-DOPA synthesis, alkene oligomerizations, water-gas shift reactions. The Reppe reaction.

Heterogeneous catalysis –The nature of heterogeneous catalysts. Alkene polymerization: Ziegler-Natta catalysis, Fischer-Tropsch carbon chain growth. New directions in heterogeneous catalysis.

Module-3

Zeolites as catalysts for organic transformation: Uses of ZSM – 5.

Alkene metathesis, hydroboration, arylation or vinylation of olefins (Heck reaction).

Biological and Medicinal Applications: Organomercury, organoboron, organosilicon and organoarsenic compounds.

Module-4

Chemistry of main group elements: Diborane and its reactions, polyhedral boranes(preparation, properties, structure and bonding). Wade's rules, carboranes andmetallocarboranes. Borazines. Phosphazenes, S-N compounds.

Metal clusters: Evidences and factors favoring of M-M bonding, Wade's-Mingo's-Lauher rules, bi, tri, tetra, penta and hexa nuclear metal carbonyl clusters. Low and high nuclearity carbonyl clusters. Electron counting schemes in carbonyl clusters. The isolobal analogy.

Module-5

Silicates: Structure, classification - silicates with discrete anions, silicates containing chainanion, silicates with layer structure, silicones with three dimensional net-work and applications.

Silicones: General methods of preparation, properties. Silicone polymers – silicone fluids, silicone greases, silicone resins, silicone rubbers and their applications.

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References

1. Organometallic Chemistry, 2nd edition, R.C. Mehrothra and A. Singh, New Age International Publications (2006).
2. Fundamental Transition Metal Organometallic Chemistry - Charles M. Lukehart, Brooks, Cole Publishing Company (1985).
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10. Chemistry of the Elements – N.N. Greenwood and A. Earnshaw, Pergamon Press (1985).
11. Inorganic Chemistry, 6th edition. D.F. Shriver, M. Weller. T. Overton, J. Rourke and F. Armastrong, Oxford University Press (2014).
12. Organometallic Chemistry and Catalysis, Didier Astruc, Springer (2007).
13. Transition Metal Organometallic Chemistry, Francois Mathey, Springer (2013).