MANONMANIAM SUNDARANAR UNIVERSITY,
TIRUNELVELI-12

SYLLABUS

PG - COURSES – AFFILIATED COLLEGES

Course Structure for M. Sc. Chemistry
(Choice Based Credit System)
(with effect from the academic year 2026-2027 onwards)

Semester-I				
Part	**Subject Status**	**Subject Title**	**Subject Code**	**Credit**
III	CORE I	ORGANIC REACTION MECHANISM-I	TCHC11	4
III	CORE II	STRUCTURE AND BONDING IN INORGANIC COMPOUNDS	TCHC12	4
III	CORE III	ORGANIC CHEMISTRY PRACTICAL - I	TCHL11	3
III	CORE IV	PHYSICAL CHEMISTRY PRACTICAL	TCHL12	3
III	ELECTIVE I	NANOMATERIALS AND NANOTECHNOLOGY	TCHE12	3
III	ELECTIVE II	ELECTROCHEMISTRY	TCHE13	3

Total Marks: 100 Internal Exam: 25 marks + External Exam: 75 marks

A. **Scheme for internal Assessment**:
Maximum marks for written test: **20 marks**
3 internal tests, each of **I hour** duration shall be conducted every semester.
To the average of the **best two** written examinations must be added the marks scored in. The **assignment** for 5 marks.

The break up for internal assessment shall be:
Written test- 20 marks; Assignment -5 marks Total - 25 marks

B. Scheme of External Examination
3 hrs. examination at the end of the semester
A – Part : 1 mark question two - from each unit
B – Part : 5 marks question one - from each unit
C – Part : 8 marks question one - from each unit

- **Conversion of Marks into Grade Points and Letter Grades**

S.No	Marks	Letter Grade	Grade point (GP)	Performance
1	90-100	O	10	Outstanding
2	80-89	A+	9	Excellent
3	70-79	A	8	Very Good
4	60-69	B+	7	Good
5	50-59	B	6	Above Average
6	40-49	C	5	Pass
7	0-39	RA	-	Reappear
8	0	AA	-	Absent

- **Cumulative Grade Point Average (CGPA)**

$$\mathbf{CGPA} = \frac{\mathbf{\Sigma\,(GP \times C)}}{\mathbf{\Sigma C}}$$

- **GP** = Grade point, **C** = Credit
- CGPA is calculated only for Part-III courses
- CGPA for a semester is awarded on cumulative basis

- **Classification**
  a) First Class with Distinction : CGPA $\geq$ 7.5*****
  b) First Class : CGPA $\geq$ 6.0
  c) Second Class : CGPA $\geq$ 5.0 and $<$ 6.0
  d) Third Class : CGPA$<$ 5.0

ORGANIC REACTION MECHANISM - I

Objectives of the course

- To understand the feasibility and the mechanism of various organic reactions.
- To comprehend the techniques in the determination of reaction mechanisms.
- To understand the concept of stereochemistry involved in organic compounds.
- To correlate and appreciate the differences involved in the various types of organic reaction mechanisms.
- To design feasible synthetic routes for the preparation of organic compounds.

UNIT-I

Methods of Determination of Reaction Mechanism: Reaction intermediates, The transition state, Reaction coordinate diagrams, Thermodynamic and kinetic requirements of reactions, Hammond postulate.

Methods of determining mechanism: Kinetic methods of determination: Rate law – Primary and secondary isotope effect. Non-Kinetic methods of determination: Testing and Trapping of intermediates, Isotopic labeling, Cross–over experiment, Product analysis and stereo chemical evidence.

Effect of structure on reactivity: Hammett and Taft equations.

UNIT-II

Aromatic and Aliphatic Electrophilic Substitution: Aromaticity: Aromaticity in benzenoid, non-benzenoid, heterocyclic compounds and annulenes.

Aromatic electrophilic substitution: Orientation and reactivity of di- and polysubstituted phenol, nitrobenzene and halobenzene. Reactions involving nitrogen electrophiles: nitration, nitrosation and diazonium coupling;

Aliphatic electrophilic substitution Mechanisms: SE2 and SEi, SE1- Mechanism and evidences.

UNIT-III

Aromatic and Aliphatic Nucleophilic Substitution:

Aromatic nucleophilic substitution: Mechanisms -SNAr, SN1and Benzyne mechanisms-Evidences- Reactivity, Effect of structure, leaving group and attacking nucleophile. Reactions: Oxygen and Sulphur-nucleophiles, Bucherer and Rosenmund reactions, Von Richter, Sommelet-Hauser and Smiles rearrangements.

Aliphatic Nucleophilic Substitution: SN1, ion pair, SN2 mechanisms and evidences. Aliphatic nucleophilic substitutions at anallylic carbon, aliphatic trigonal carbon and vinyl carbon. SN1' SN2' and SNi' mechanism and evidences,-Ambident nucleophiles.

UNIT-IV

Stereochemistry-I: Introduction to molecular symmetry and chirality – axis, plane, center, alternating axis of symmetry. prochirality, enantiotopic and diastereotopic atoms, groups, faces, axialand planar chirality, chiralitydue to helical shape, methods of determining the configuration.

Racemic modifications: Racemization by thermal, anion, cation, reversible formation, epimerization, mutarotation. D, L system, Cram's and Prelog's rules: R, S-notations, proR, proS, side phase and re phase Cahn-Ingold-Prelogrules,absoluteandrelativeconfigurations.Configurationsofallenes, spiranes, biphenyls, cyclooctene, helicene, binaphthyls, ansa and cyclophanic compounds, asymmetric synthesis, destruction.

UNIT-V

Stereochemistry-II:

Curtin-Hammett Principle. Stability of five and six-membered rings: mono-,di and Poly substituted cyclohexanes, conformation and reactivity in cyclohexane systems. Fused and bridge drings: bicyclic, polycyclic systems, decalins and Brett's rule.

Optical rotation and optical rotatory dispersion, conformational asymmetry, ORD curves, octant rule, configuration and conformation, Cotton effect, axial haloketone rule and determination of configuration.

Recommended Text

1. J.MarchandM.Smith,AdvancedOrganicChemistry,5thedition,John- Wiley and Sons.2001.
2. E.S.Gould,MechanismandStructureinOrganicChemistry,Holt, Rinehart and Winston Inc., 1959.
3. P.S.Kalsi,Stereochemistryofcarboncompounds,8thedition,NewAge International Publishers, 2015.
4. P.Y.Bruice, OrganicChemistry,7thedn,Prentice Hall, 2013.
5. J.Clayden,N.Greeves,S.Warren,OrganicCompounds,2ndedition, Oxford University Press, 2014.

Reference Books

1. F.A.Carey andR.J.Sundberg,AdvancedOrganicChemistry Part-A and B, 5th edition, Kluwer Academic / Plenum Publishers, 2007.
2. D.G.Morris, Stereochemistry, RSCTutorialChemistryText1,2001.
3. N.S.Isaacs,PhysicalOrganicChemistry,ELBS,Longman,UK,1987.
4. E.L.Eliel,StereochemistryofCarbonCompounds,Tata-McGrawHill, 2000.
5. I.L.Finar,Organicchemistry,Vol-1&2,6thedition,PearsonEducation Asia,2004.

Website and e-learning source

1. https://sites.google.com/site/chemistryebookscollection02/home/organicchemistry/organic
2. https://www.organic-chemistry.org/

STRUCTURE AND BONDING IN INORGANIC COMPOUNDS

UNIT I - CHEMICAL BONDING

Valence Bond theory: Lewis structure – Concepts and VB theory of H_2 molecule - Stereochemistry of hybrid orbitals – Calculation of s and p Characters of equivalence and nonequivalence of hybrid orbitals-VSEPR theory.

M.O. theory – Linear combination of Atomic orbitals (s – s, s – p, d – p, p – p and d –doverlapping) – σ ,π ,δ and quadruple bond. – M.O. diagrams of hetero nuclear diatomic molecules (CO, NO, HF) and triatomic molecules (BeH2,H2O,CO2)–Walsh diagrams–Structure and hybridization - Bents rule and apicophilicity.

Ionic Bond: Lattice energy-Born-Lande equation, Born Haber cycle and Kapustinskii equation.

UNIT - II: Structure of main group compounds and clusters:

Structure of silicates - applications of Pauling's rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three-dimensional silicates. Structure of silicones, Structural and bonding features of B-N, S-N and P-N compounds; Poly acids – types, examples and structures; Borane cluster: Structural features of closo, nido, arachano and klado; carboranes, hetero and metallo boranes; Wade's rule to predict the structure of borane cluster; main group clusters–zintl ions.

UNIT-III: Solid state chemistry – I: Ionic crystals: Packing of ions in simple, hexagonal and cubic close packing, voids in crystal lattice, Radius ratio, Crystal systems and Bravais lattices, Symmetry operations in crystals, glide planes and screw axis; point group and space group. X-ray diffraction technique: Bragg's law, Powder diffraction method– Principle and Instrumentation.

UNIT-IV: Solid state chemistry – II: Structural features of the crystal systems: Rock salt, zinc blende & wurtzite, fluorite and anti-fluorite, rutile and anatase, cadmium iodide and nickelarsenide;Spinels –normal and inverse types and perovskite structures. Crystal Growth methods: From melt and solution (hydrothermal, sol-gelmethods)– principles and examples.

UNIT- V: Band theory and defects in solids

Band theory – features and its application of conductors, insulators and semiconductors, Intrinsic and extrinsic semiconductors; Defects in crystals – point defects (Schottky, Frenkel, metal excess and metal deficient) and their effect on the electrical and optical property; Linear defects and its effects due to dislocations and colour centers.

Recommended Text

1. ARWest,SolidstateChemistryand itsapplications,2ndEdition (Students Edition), John Wiley & Sons Ltd., 2014.
2. A K Bhagi and G R Chatwal, A textbook of inorganic polymers, Himalaya Publishing House, 2001.
3. L Smart, E Moore, Solid State Chemistry – An Introduction, 4th Edition, CRC Press, 2012.
4. K. F. Purcelland J. C. Kotz, Inorganic Chemistry; W.B. Saunders company: Philadelphia, 1977.
5. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry; 4th ed.; Harper and Row: NewYork, 1983.

Reference

1. Books 1. D.E.Douglas,D.H.McDanielandJ.J. Alexander,Conceptsand Models in Inorganic Chemistry, 3rd Ed, 1994.
2. RJDTilley, Understanding Solids - The Science ofMaterials, 2nd edition, Wiley Publication, 2013.
3. CNR Rao and J Gopalakrishnan, New Directions in Solid State Chemistry, 2nd Edition, Cambridge University Press, 199.
4. T.Moeller,InorganicChemistry,AModernIntroduction;John Wiley: New York, 1982.
5. D.F.Shriver,P.W.AtkinsandC.H.Langford;Inorganic Chemistry; 3rd ed.; Oxford University Press: London, 2001.

Website and e-learning source

1. https://ocw.mit.edu/courses/3-091-introduction-to-solid-state-chemistryfall-2018/video_galleries/lecture-videos/

ORGANIC CHEMISTRY PRACTICAL - I

A. **Qualitative analysis of Organic mixture** (atleast six two component mixtures):

- Separation of organic mixtures
- Elemental analysis
- Functional group(s) identification
- Preparation of derivatives
- Physical properties determination (melting point and boiling point) for both components and their derivatives.

Analysis may be performed in micro (or) macro scale depending upon the conditions of the laboratory.

B. **For Classwork:**

Three component mixtures (Separation)

Recommended Text

1. A.I.Vogel,ElementaryPracticalOrganic Chemistry:SmallScale Preparations, Qualitative Organic Analysis, Quantitative Organic Analysis, Pearson Education, 2011.
2. K.Bansal Raj, Laboratory Manual of Organic Chemistry, New AgeInternational, 2009.
3. V.Venkateswaran,R.VeeraswamyandA.R.Kulandaivelu,Basic Principles of Practical Chemistry, Sultan Chand & Sons, 2004.
4. V.K. Ahluwalia, and R. Aggarwal, Comprehensive Practical Organic Chemistry, Universities Press, 2004

Reference Books

1. R.G. Engel, D.L. Pavia, G.M. Lampman and G.S. Kriz, A Microscale approach to Organic Laboratory, 5th edition, Paperback – International Edition, 2012.
2. P.B. Cranwell, L.M. Harwood, and C. J. Moody, Experimental Organic Chemistry, 3rd edn,Wiley-Blackwell, 2017.
3. J. Leonard,B.Lygo and G. Procter, Advanced PracticalOrganic Chemistry, 3rd edn, CRC Press, 2013.

Website and e-learning source

1. https://ocw.mit.edu/courses/3-091-introduction-to-solid-statechemistry-fall-2018/video_galleries/lecture-videos/

PHYSICAL CHEMISTRY PRACTICAL

UNIT-I: Conductivity Experiments

1. Determination of equivalent conductance of a strong electrolyte & the verification of DHO equation.
2. Verification of Ostwald's Dilution Law & Determination of pKa of a weak acid.
3. Verification of Kohlrausch's Law for weak electrolytes.
4. Determination of the equivalent conductance of a weak acid at different concentrations and verifying Ostwald dilution law.
5. Calculation of the dissociation constant of the acid. Determination of the equivalent conductance of a strong electrolyte at different concentrations and examining the validity of the Onsager's theory as limiting law at high dilutions.
6. Conductometric titration of a mixture of HCl and CH_3COOH Vs NaOH.
7. Conductometric titration of NH_4Cl Vs NaOH.
8. Conductometric titration of CH_3COONa Vs HCl.

UNIT-II: Kinetics

1. Study the kinetics of acid hydrolysis of an ester; determine the temperature coefficient and also the activation energy of there action.

2. Study the kinetics of the reaction between acetone and iodine in acidic medium by half-life method and determine the order with respect to iodine and acetone.

UNIT-III: Phase diagram

Construction of phase diagram for a simple binary system

1. Naphthalene-phenanthrene
2. Benzophenone-diphenylamine.

Recommended Text

1. B.ViswanathanandP.S.Raghavan,PracticalPhysicalChemistry, Viva Books, New Delhi, 2009.
2. Sundaram,Krishnan,Raghavan,PracticalChemistry(PartII),S. Viswanathan Co. Pvt., 1996.
3. V.D. Athawale and Parul Mathur, Experimental Physical Chemistry, New Age International (P) Ltd., New Delhi, 2008.
4. E.G.Lewers, Computational Chemistry: Introduction to the Theory and Applications ofMolecularandQuantumMechanics,2ndEd., Springer, New York, 2011.

Reference Books

1. J.B.Yadav,AdvancedPractical Physical Chemistry,Goel Publishing House, 2001.
2. G.W.Garland,J.W.Nibler,D.P.Shoemaker,Experimentsin Physical Chemistry, 8th edition, McGraw Hill, 2009.
3. J.N.GurthuandR.Kapoor,AdvancedExperimentalChemistry,S. Chand and Co., 1987.
4. ShailendraKSinha,PhysicalChemistry:AlaboratoryManual,Narosa Publishing House Pvt, Ltd., New Delhi, 2014.
5. F.Jensen,IntroductiontoComputational Chemistry,3rdEd.,Wiley- Blackwell.

Website and e-learning source

1. https://web.iitd.ac.in/~nkurur/2015-16/Isem/cmp511/lab_handout_new.pdf

NANOMATERIALS AND NANO TECHNOLOGY

UNIT-I: Introduction of nanomaterials and nanotechnologies:

Introduction-roleofsize,classification-0D,1D,2D,3D.consolidationof Nano powders. Features of nanostructures, Background of nanostructures. Techniques of synthesis of nanomaterials- Bottom–Up, Top–Down, Tools of the nanoscience. Applications of nanomaterials and technologies.

UNIT-II: Synthetic Methods: Bonding and structure of the nanomaterials, Predicting the Type of Bonding in a Substance crystal structure. Metallic nanoparticles, Surfaces of Materials, Nanoparticle Size and Properties. Synthesis-Physical and chemical

method s- inertgas condensation, arc discharge, laser ablation, sol-gel, solvothermal and hydrothermal-CVD-types, metalloorganic, plasma enhanced, and low pressure CVD. Microwave assisted and electrochemical synthesis.

UNIT-III: Mechanical Properties of Nanomaterials: Mechanical properties of materials, theories relevant to mechanical properties. Techniques to study mechanical properties of nanomaterials, adhesion and friction, thermal properties of nanomaterials Nanoparticles: gold and silver, metaloxides: silica, ironoxide and alumina- synthesis and properties.

UNIT-IV: Electrical Properties of Nanomaterials: Electrical properties, Conductivity and Resistivity, Classification of Materialsb based on Conductivity, magnetic properties, electronic properties of materials. Classification of magnetic phenomena. Semiconductor materials – classification-Ge, Si, GaAs, SiC, GaN, GaP, CdS, PbS. Identification of materials as p and n –type semiconductor-Hall effect – quantum and anomalous, Hall voltage- interpretation of charge carrier density. Applications of semiconductors: p-njunction as transistors and rectifiers, photovoltaic and photogalvanic cell.

UNIT-V: Nano Composites: Nanothinfilms, nanocomposites. Application of nanoparticles in different fields. Core-shell nanoparticles - types, synthesis, and properties. Nanocomposites - metal- ceramic- and polymer-matrix composites-applications.
Characterization–SEM, TEM and AFM-principle, instrumentation and applications.

Recommended Text

1. S.MohanandV.Arjunan,PrinciplesofMaterialsScience,MJP Publishers, 2016.
2. Arumugam,MaterialsScience,AnuradhaPublications,2007.
3. Giacavazzoet.al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010
4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.
5. JamesF. Shackelford and MadanapalliK.Muralidhara,Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.

Reference Books

1. S.Mohanand V.Arjunan,PrinciplesofMaterialsScience,MJP Publishers, 2016.
2. Arumugam,MaterialsScience,AnuradhaPublications,2007.
3. Giacavazzo et.al., Fundamentals of Crystallography, International Union of Crystallography. Oxford Science Publications, 2010
4. Woolfson, An Introduction to Crystallography, Cambridge University Press, 2012.

5. James F. Shackelford and Madanapalli K. Muralidhara, Introduction to Materials Science for Engineers. 6th ed., PEARSON Press, 2007.

Website and e-learning source

1. http://xrayweb.chem.ou.edu/notes/symmetry.html.
2. http://www.uptti.ac.in/classroom-content/data/unit%20cell.pdf.

ELECTROCHEMISTRY

UNIT - I: Ionics: Arrhenius theory-limitations, Van't Hoff factor and its relation to colligative properties. Deviation from ideal behavior. Ionic activity, mean ionic activity and mean ionic activity coefficient-concept of ionic strength, Debye Huckel theory of strong electrolytes, activity coefficient of strong electrolytes. Determination of activity coefficient ion-solvent and ion-ion interactions. Derivation of Debye-Huckel limiting law at appreciable concentration of electrolytes modifications and applications. Electrolytic conduction-Debye-Huckel Onsager treatment of strong electrolyte – qualitative and quantitative verification and limitations.

UNIT-II: Electrode-electrolyte interface: Interfacial phenomena - Evidences for electrical double layer, polarizable and non-polarizable interfaces, Electrocapillary phenomena - Lippmann equation electro capillary curves. Electro-kinetic phenomena electro-osmosis, electrophoresis, streaming and sedimentation potentials, colloidal and poly electrolytes. Structure of double layer: Helmholtz -Perrin, Guoy- Chapman and Stern models of electrical double layer. Zeta potential and potential at zero charge. Applications and limitations.

UNIT - III: Electrodics of Elementary Electrode Reactions: Behavior of electrodes: Standard electrodes and electrode sat equilibrium. Anodic and Cathodic currents, condition for the discharge of ions. Nernst equation, polarizable and non-polarizable electrodes. Model of three electrode system, over potential. Rate of electro chemical reactions: Rates of simple elementary reactions. Butler-Volmer equation and Tafel equation-significance of exchange current density, net current density and symmetry factor. Low and high field approximations. Symmetry factor and transfer coefficient Tafel equations and Tafel plots.

UNIT-IV: Electrodics of Multistep Multi Electron System: Rates of multi-step electrode reactions. Rate determining step, electrode polarization and depolarization. Transfer coefficients, its significance and determination, Stoichiometric number. Reduction of I3-, Fe2+ and dissolution of Fe to Fe2+. Overvoltage - Chemical and electro chemical, Phase, activation and concentration over potentials. Evolution of oxygen and hydrogen at different pH. Pourbiax and Evan's diagrams.

UNIT-V: Concentration Polarization, Batteries and Fuel cells: Modes of Transport of electro active species - Diffusion, migration and hydrodynamic modes. Role of supporting electrolytes. Polarography principle and applications. Cyclic voltammetry-anodic and cathodic stripping voltammetry and differential pulse voltammetry. Sodium and lithium-ion batteries and redox flow batteries.
Energy production systems: Fuel Cells: classification, alkaline fuel cells, phosphoric acid fuel cells, high temperature fuel cells.

Recommended Text

1. D.R.Crow,Principlesandapplicationsofelectrochemistry, 4thedition, Chapman & Hall/CRC, 2014.
2. J.RajaramandJ.C.Kuriakose,KineticsandMechanismofchemical transformations Macmillan India Ltd., New Delhi, 2011.
3. S.Glasstone,Electrochemistry,AffiliatedEast-WestPress,Pvt., Ltd., New Delhi, 2008.
4. B.Viswanathan,S. Sundaram,R. Venkataraman,K. Rengarajan and P.S.Raghavan, Electrochemistry-Principlesandapplications,S. Viswanathan Printers, Chennai,2007.
5. JosephWang, Analytical Electrochemistry, 2nd edition, Wiley,2004.

Reference Books

1. J.O.M.BockrisandA.K.N.Reddy,ModernElectrochemistry,vol.1 and 2B, Springer, Plenum Press, New York, 2008.
2. J.O.M.Bockris,A.K.N. Reddy and M.G.AldecoMorden Electro chemistry, vol. 2A, Springer, Plenum Press, New York, 2008.
3. PhilipH.Rieger,Electrochemistry,2ndedition,Springer,NewYork, 2010.
4. L.I.Antropov,Theoreticalelectrochemistry,MirPublishers, 1977.
5. K.L.Kapoor,ATextbookofPhysicalchemistry,volume-3, Macmillan, 2001.

Website and e-learning source

1. https://www.pdfdrive.com/modern-electrochemistry-e34333229