M.SC.,
PHYSICAL CHEMSITRY

MODEL SYLLABUS

AUGUST- 2022

TAMILNADU STATE COUNCIL FOR HIGHER EDUCATION,
CHENNAI – 600 005

M.Sc.,
PHYSICAL CHEMISTRY

Programme:	**M.Sc. PHYSICAL CHEMISTRY**
Programme Code:	**CHE**
Duration:	**TWO years**
Programme Outcomes:	After completion of this M.Sc. Physical Chemistry program, the students will be able to: • **PO-1:** Demonstrate comprehensive knowledge and skills in M.Sc. Physical Chemistry along with Organic, Inorganic, analytical and Materials Chemistry and other modern areas of Chemistry. • **PO-2:** Apply knowledge and experimental skills to synthesize and analyze chemicals/ materials of immediate need for the society and relevance to chemical and allied industries. • **PO-3:** Employ advanced tools, techniques, and methodologies to achieve the evidence-based solutions for local and global problems related to Physical Chemistry. • **PO-4:** Apply disciplinary knowledge and transferable skills in the interdisciplinary areas of chemistry to solve problems with well-defined solutions. • **PO-5:** Critically evaluate practices, rules, and theories based on empirical evidence, by following the scientific approach to knowledge development in PhysicalChemistry. • **PO-6:** Develop benchmark standards in writing, communications, team-work, and ethics to disseminate results of studies undertaken in Physical Chemistry. • **PO-7:** Prepare for self-learning and lifelong-learning to meet one's learning needs using research and development work and professional materials. • **PO-8:** Demonstrate knowledge and transferable skills in cutting-edge-areas of Physical Chemistry that empower them for employment opportunities in academia, research laboratories, chemical and allied industries. • **PO-9:** Demonstrate ability to work effectively with diverse teams, facilitate cooperative effort as a member or leader of a team to achieve the deliverables of any project. • **PO-10:** Demonstrate knowledge of the values of multiple cultures and a global perspective effectively engage in a multicultural society for employment or further studies.
Programme Specific Outcomes:	After the completion of this M.Sc. Physical Chemistry program, the student will be able to: • **PSO-1:** Demonstrate comprehensive knowledge and skills in Physical Chemistry along with different areas of Chemistry, viz; Organic, Inorganic, Analytical and Materials Chemistry.

	• **PSO-2:** Apply knowledge and experimental skills to synthesize and analyze chemicals/ materials of immediate need for the society and relevance to chemical and allied industries. • **PSO-3:**Critically evaluate practices, rules,and theories based onempirical evidence, by following the scientific approach to knowledge development in PhysicalChemistry. • **PSO-4:** Demonstrate effective communication skills both orally and in writing using appropriate media in all the aspects related to Chemistry andone's profession. • **PSO-5:** Demonstrate a sense of inquiry and ability to define problems; use research methods, analyze, interpret and draw conclusions from data; plan, execute and report the results of an experiment or investigation in intra/interdisciplinary areas of chemistry.

List of Courses:

Semester	Course Code	Title of the Course	Core/Elective/ Soft Skill	Credits
SEMESTER - I				
I	CHE C001	Fundamentals of Analytical Chemistry	Core	3
I	CHE C101	Coordination and Nuclear Chemisty	Core	3
I	CHE C201	Stereochemistry and Organic Reaction Mechanism	Core	3
I	CHE C301	Thermodynamics, Electrochemisty and Chemical Kinetics	Core	3
I	CHE C202	Organic Chemisty Practical – I	Core	3
I	CHE C302	Physical Chemistry Practical – I	Core	3
SEMESTER - II				
II	CHE C002	Analytical Instrumentation	Core	3
II	CHE C102	Main Group Elements and Inorganic Polymers	Core	3
II	CHE C203	Organic Reaction Mechanism	Core	3
II	CHE C303	Quantum Chemistry and Group Theory	Core	3
II	CHE C003	Analytical Chemisty Practical – I	Core	3
II	CHE C103	Inorganic Chemisty Practical – I	Core	3
SEMESTER - III				
III	CHE C601	Physical Methods in Chemistry	Core	4
III	CHE C304	Physical Chemistry Practical – II	Core	3
III	CHE C305	Physical Chemistry Practical – III	Core	3
III	CHE C309	Advanced materials for catalysis and drug delivery applications	Core	4
III	CHE C510	Electrochemical Energy Device	Core	4
SEMESTER - IV				
IV	CHE C306	Advanced Thermodynamics and Kinetics of Chemical Reactions and Electrochemistry	Core	4

IV	CHE C307	Advanced Quantum Chemistry and Applied Materials	Core	4
IV	CHE C308	Project	Core	6
	Elective & Soft Skill Courses Offered for the Department/ School			
I	CHE E001	Electronics and Computers for Chemists	Elective	3
I	CHE E101	Inorganic Reaction Mechanism	Elective	3
I	CHE E201	Name Reactions in Organic Chemistry	Elective	3
I	CHE E301	Essentials of Statistical Thermodynamics	Elective	3
I	UOMS147	Software packages for Chemists – MATLAB, ORIGIN AND CHEMDRAW	Soft Skill	2
I	UOMS115	Lab Safety and First Aid	Soft Skill	2
II	CHE E002	Analysis of Complex Materials	Elective	3
II	CHE E102	Nuclear Chemistry	Elective	3
II	CHE E202	Functional Group Transformation in Organic Chemistry	Elective	3
II	CHE E302	Macromolecular Chemistry – I	Elective	3
II	UOMS116	Fire Safety and Firefighting	Soft Skill	2
III	CHE E601	Biological Chemistry	Elective	3
III	CHE E602	Photochemistry and Nanomaterials	Elective	3
III		Elective (from other school)	Elective	3
III	UOMS117	Chemistry Databases- Scifinder, Mandeleef, Scopus, Web of Science and Google Scholar	Soft Skill	2
III	UOMS118	Spectroscopy Instrumentation	Soft Skill	2
III	UOM1001	Internship	Internship	2
IV	CHE E004	Electro Analytical Chemistry	Elective	3
IV	CHE E005	Introduction to Chromatography and Surface Techniques	Elective	3
IV	CHE E603	Novel Reagents in Organic Synthesis	Elective	3
IV	UOMS119	Glass Blowing Techniques	Soft Skill	2
IV	CHE E303	Macromolecular Chemistry – II	Elective	3

Scheme:

Courses	**Number of Minimum Credits required for the award of Degree**
Core	60
Elective	21
Soft Skill	08
Internship	02
Total	**91**

Method of Evaluation:

Courses	Sessional I	Sessional II	End Semester Examination	Total Marks	Range of Marks	Letter of Grade
Core Theory/ Soft Skill/ Project/ Internship	20	20	60	100	90-100 80-89 75-79 70-74 60-69 50-59 ABSENT	O D+ D A+ A B AAA
Core Practicals	-	-	50	50		

SEMESTER – I

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	CHE C301	Thermodynamics, Electrochemistry and Chemical Kinetics	3

Course Objectives:

The main objectives of this course are,

- To provide basics and knowledge related to thermodynamics in terms of system, chemical potential and phase equilibria.
- To understand theories and principles of electrochemistry in terms of electrolytic conductance, electrode equilibrium and electromotive force.
- To learn kinetic theories and factors affecting reaction rates, complex reactions, fast reactions and adsorption reactions.
- To correlate and apply the fundamental knowledge in thermodynamics, electrochemistry and chemical kinetics to different areas of chemistry and emerging problems in basic science.
- To demonstrate the ability to do some independent research and use some experimental resources at the end of the course.

Pre-requisites, if any:

Students should know the UG level fundamental aspects on thermodynamics, electrochemistry and chemical kinetics along with problems solving.

Course Outcomes:

After completion of this course successfully, the students will be able to..

- **CO1:** Recall basics of thermodynamics, electrochemistry and chemical kinetics. (**K1**)
- **CO2:** Understand the relationships of thermodynamics, electrochemistry and chemical kinetics in chemical reaction dynamics. (**K2**)
- **CO3:** Apply the knowledge of thermodynamics, electrochemistry and chemical kinetics to different areas of chemistry. (**K3**)
- **CO4:** Analyze and Evaluate research problems in thermodynamics, electrochemistry and chemical kinetics. (**K4** and **K5**).
- **CO5:** Create new concepts to give contribution to dimensional growth for thermodynamics, electrochemistry and chemical kinetics. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6**– Create

UNITS

UNIT - I: Kinetic Theory and Thermodynamics **(10 Hours)**

Thermodynamic description of various types of process, Laws, state and path function Second law of thermodynamics, Maxwell's relations and thermodynamic equations of state, (C_P-C_V) in terms of coefficient of expansion and coefficient of compressibility.

Closed and open systems, partial molal quantities and experimental determination, chemical potential, Gibbs-Duhem and Gibbs-margules equation, variation of chemical potential with temperature and pressure.

Real systems, fugacity and activity, activity coefficients and their electrochemical and graphical determination, standard states for gases, liquids, solids and solutions, Lewis – Randall rule and its applications.

Phase Equilibria Thermodynamic derivation of phase rule – application to three component systems of

(1) Acetic acid, chloroform and water

(2) Ammonium chloride, ammonium sulphate and water.

UNIT - II: Electrochemistry-I (9 Hours)

Nernst Equation, Redox System, Electrolytic conductance of Kohlrausch's law and it is Applications. Theory of electrolytic dissociation – ionic activity and activity coefficients, Debye -Huckel-Onsagar theory of interionic attraction and its refinements. Influence of ionic atmosphere on the conductivity of electrolytes, equation for the equivalent conductivity of electrolytes – Experimental verification of the equation. Electrode equilibrium - Thermodynamics, electrodes and electrode potentials, electrochemical cells, electromotive force.

UNIT - III: ELECTROCHEMISTRY-II (8 Hours)

Polarization and overpotential – concentration polarization – Polarography. Electrochemical polarization – Butler – Volmer equation for one electron transfer reaction and Tafel equations. Ionic equilibria – conductometric and potentiometric titrations.

UNIT - IV: Chemical Kinetics (10 Hours)

Mechanisms of complex reactions – equilibrium and steady state approximation; Theories of reaction rates - collision theory, transition state theory and its thermodynamic aspects - enthalpy, entropy and free energy of activations; Kinetics of complex reactions - opposing, parallel and consecutive reactions; Unimolecular reactions; Kinetic isotopic effects; Salt effects; Potential energy surfaces and reaction coordinates. Factors determining reaction rates in solution - solvent, dielectric constant and ionic strength; Fast reactions - T-jump, flow methods, pump-pulse, relaxation methods.

UNIT – V: Adsorption and Colloids (8 Hours)

Langmuir, Freundlich, BET and Gibbs adsorption isotherms; Surface films; Homogeneous and Heterogeneous catalysis; Reactions on surfaces - Simple decomposition, Bimolecular reactions by Langmuir-Hinshelwood and Eley-Rideal mechanisms.

Surface tension, viscosity. Self-assembly. Physical chemistry of colloids and micelles.

Reference Books:

1. Thermodynamics for chemists, S. Glasstone, Affiliated East West
2. Chemical Thermodynamics, I. M. Klotz and R. M. Rosenberg, Benjamin, Menlo Park, 1972.
3. Thermodynamics, J. C. Kuriakose, J. Rajaram.
4. An Introduction to Electrochemistry, S. Glasstone, An East West Edition.
5. Modern Electrochemistry Vol. I J. O' M Bockris and A. K. N. Reddy, Plenum, New York, 1970.
6. Theoretical Electrochemistry, LI. Antropov, Mir. Publication.
7. Chemical Kinetics, K. J. Laidler, 2nd Ed, McGraw Hill.
8. Kinetics and mechanism, John. W. Moore, Ralph. G. Pearson, 3rd Ed, Wiley, 1981

Text Books:

1. Physical Chemistry, G. M. Barrow, 4 th Ed., McGraw Hill.
2. Physical Chemistry, P. W. Atkins, 4 th Ed., Oxord.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://www.youtube.com/watch?v=S73srEM_4QA&list=PL9m2Lkh6odgK6pbaO7Yddu_jPzYlK8OM5
2. https://www.youtube.com/watch?v=yrnQTAc_S8o
3. https://www.youtube.com/watch?v=PH1DR0c-jqw
4. https://www.youtube.com/watch?v=dNkDAgg9MUY
5. https://www.youtube.com/watch?v=pm3HpBfooMA
6. https://www.youtube.com/watch?v=XaId7WR0mGo

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	S	M	L	M	M	S	S	S	M
CO 2	M	S	S	M	S	L	M	L	S	M
CO 3	M	M	L	S	S	M	M	S	S	S
CO 4	M	S	L	S	M	M	L	S	L	M
CO 5	S	M	M	S	M	L	L	M	S	S

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C302**	**Physical Chemistry Practical – I**	**3**

Course Objectives:

The main objectives of this course are,

- To provide experimental knowledge on adsorption isotherm and heat of neutralization.
- To understand the applications of conductivity experiments to determine solubility product, neutralization point, weak and strong electrolyte behavior.
- To recognize the applications of EMF measurements to determine pH of a solution and solubility product.
- To demonstrate the reaction kinetics of ester hydrolysis, simple eutectic system and equilibrium in solutions.
- To develop the ability to do some independent experiments and learn recent developments inthe related experiments at the end of the course.

Pre-requisites, if any:

Students should know the UG level fundamentals of physical chemistry practicals like solution preparation, normality, molarity, solution dilution, etc.

Course Outcomes:

After completion of this course successfully, the students will be able to..

- **CO1:** Recall the basics and practices of physical chemistry practicals. **(K1)**
- **CO2:** Understand the experimental aspects of different areas of physical chemistry. (**K2**)
- **CO3:** Apply the knowledge of experimental physical chemistry to existing and emerging problems in basic sciences. (**K3**)
- **CO4:** Analyze and Evaluate the research problems in different areas of physical chemistry. (**K4** and **K5**).
- **CO5:** Create new concepts to expand the dimensions of the experimental physical chemistry. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

Experiments **(135 Hours)**

1. Adsorption- verification of Freundlich adsorption isotherm
2. Thermochemistry – heat of neutralization of a strong acid
3. Conductivity
   (a) Cell constant determination
   (b) Solubility product of a sparingly soluble salt
   (c) Acid – base titration(strong acid vs strong base; strong base vs weak acid) ,precipitation titration(barium chloride vs magnesium sulphate)
   (d) Dissociation constant of a weak acid- verification of Ostwald's dilution law
   (e) Verification of Onsager equation- strong electrolyte
4. EMF
   (a) Determination of buffer and pH-quinhydrone electrode- Henderson's relation
   (b) Determination of solubility product of sparingly soluble AgX type salts.
5. Reaction kinetics
   Hydrolysis of ester- comparison of strength of acids, determination of hydrolysis constant.
6. Phase rule and thermodynamics
   Simple eutectic
7. Equilibrium in solutions
   (a) Association factor of benzoic acid in benzene and water
   (b) $KI + I_2 = KI_3$. Equilibrium constant in aqueous media

Text Books:

1. D.P. Shoemaker and C.W.Garland, Experiments in Physical Chemistry, McGraw Hill, 1962.
2. Findlay's Practical Physical Chemistry, Longman, 1954
3. An Introduction to Electrochemistry, S. Glasstone, an East West Edition.

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	M	S	M	M	S	S	L	M	S
CO 2	M	M	M	M	S	M	M	S	M	L
CO 3	S	S	S	L	M	L	S	S	L	M
CO 4	M	S	S	S	M	S	L	M	S	M
CO 5	M	S	M	S	M	L	M	S	M	S

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Elective	**CHE E301**	**Essentials of Statistical Thermodynamics**	**3**

Course Objectives:

The main objectives of this course are,

- To provide basics of statistical thermodynamics in terms of concept of distribution, probability, ensemble and microstates.
- To learn the concepts of partition functions and its applications to calculate thermodynamic properties.
- To study different concepts of statistics and apply to electrons in metal to helium.
- To correlate the fundamental knowledge in statistical thermodynamics with different areas of chemistry and emerging problems in basic sciences.
- To develop the ability to do some independent research problems and use some experimental resources at the end of the course.

Pre-requisites, if any:

Students should know the UG level fundamental aspects on thermodynamics and statistical thermodynamics along with problems solving.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall basics and principles of statistical thermodynamics. (**K1**)
- **CO2:** Understand the importance of statistical thermodynamics in chemical reaction dynamics. (**K2**)
- **CO3:** Apply the knowledge of statistical thermodynamics to different areas of chemistry. (**K3**)
- **CO4:** Analyze and Evaluate research problems in statistical thermodynamics. (**K4** and **K5**).
- **CO5:** Create new concepts to expand the dimensions of in statistical thermodynamics. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6**- Create

UNITS

UNIT - I: Basics of Statistical Thermodynamics **(9 Hours)**

A Review of Thermodynamics and Kinetic theory of gases. Phase space. Ensemble. Liouville theorem. Equal a priori probability. Microcanonical ensemble. Quantization of phase space. Classical limit. Various distributions using Microcanonical ensemble.

UNIT - II: Probability Factor **(9 Hours)**

Concept of distribution, thermodynamic probability and most probable distribution. Ensembles, Canonical, grand canonical, micro canonical ensembles.

UNIT - III: Partition Functions **(9 Hours)**

Partition functions - translational, rotational, vibrational and electronic: calculation of thermodynamic properties ΔS, ΔS, ΔG, ΔU, ΔH, C_v, in terms of partition functions.

UNIT - IV: Types of Statistics **(9 Hours)**

Equilibrium constants and rare constants in terms of partition functions: Fermi-Dirac (FD), Maxwell, Boltzmann. Bose-Einstein (BE) statistics: Application to electrons in metals (FD), and to helium (BE).

UNIT - V: Fluctuations **(9 Hours)**

Mean square deviation and fluctuation in ensembles. Concentration fluctuation in quantum statistics. Non-equilibrium States-Boltzmann transport equation. Particle diffusion. Electrical conductivity

Reference books:

1. Thermodynamics - J. Rajaraman, SC Kuriakose, SLN Chand, 1986.
2. Physical chemistry - PW Atkins, Oxford, 5th ed., 1995.
3. B.K. Agarwal and M. Eisner, Statistical Mechanics, (1988) Wiley Eastern, New Delhi.
4. D.A. McQuarrie, Statistical mechanics, (1976) Harper and Row Publishers, New York.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://www.youtube.com/watch?v=4RX_lpoGRBg&list=PLUl4u3cNGP60gl3fdUTKRrt5t_GPx2sRg
2. https://www.youtube.com/watch?v=w_I0AkvbWFc&list=PLUl4u3cNGP60gl3fdUTKRrt5t_GPx2sRg&index=5
3. https://www.youtube.com/watch?v=BwIUE1C6Iwk
4. https://www.youtube.com/watch?v=XIXQ38JnF0k
5. https://www.youtube.com/watch?v=LIbjB2Tef8A
6. https://www.youtube.com/watch?v=KBe1d8BdjqQ

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO 5**	**PO 6**	**PO 7**	**PO 8**	**PO 9**	**PO 10**
CO 1	M	S	S	S	M	S	M	M	M	S
CO 2	S	M	S	M	S	M	M	M	L	M
CO 3	M	S	L	L	M	S	L	S	M	M
CO 4	M	S	M	S	S	M	S	M	S	M
CO 5	S	M	L	M	M	S	M	L	M	S

SEMESTER – II

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C303**	**Quantum Chemistry and Group Theory**	**3**

Course Objectives:

The main objectives of this course are,

- To provide the fundamentals of quantum chemistry in terms of Schrodinger equation, simple harmonic oscillator, rigid rotator, bonding in molecules.
- To understand group theory in terms point group of a molecule and its applications to spectral transitions.
- To learn the principles of microwave, IR and Raman spectroscopy with application to different molecules.
- To correlate and apply the fundamental knowledge of quantum chemistry, group theory and spectroscopy to the different areas of chemistry.
- To develop the ability to do some independent calculations and use some theoretical concepts at the end of the course.

Pre-requisites, if any:

Students should know the UG level fundamental aspects on quantum chemistry, group theory and spectroscopy along with problems solving.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall basics of quantum chemistry, group theory and spectroscopy. (**K1**)
- **CO2:** Understand the relationships of quantum chemistry, group theory and spectroscopy. (**K2**)
- **CO3:** Apply the knowledge of quantum chemistry, group theory and spectroscopy to different problems in chemistry. (**K3**)
- **CO4:** Analyze and Evaluate problems of quantum chemistry, group theory and spectroscopy. (**K4** and **K5**).
- **CO5:** Create new concepts to expand the dimensions of quantum chemistry, group theory and spectroscopy. (**K6**)

K1 - Remember; **K2 -** Understand; **K3 -** Apply; **K4 -** Analyze; **K5 -** Evaluate; **K6** – Create

UNITS

UNIT - I: Quantum Chemistry-I **(10 Hours)**

Blackbody radiation, Photoelectric effect, Bohr's quantum theory, Wave Particle duality uncertainty principle. Operator Algebra – linear and Hermitionan operators, Quantum mechanical postulates, Schrodinger equation and its solutions to the problem of a particle in one and three dimensional boxes, Quantum mechanical results for a simple harmonic oscillator and rigid rotator. Schrodinger equation for the hydrogen atom and its solution, the origin of electronic quantum numbers and their physical significance.

UNIT - II: Quantum Chemistry-II **(8 Hours)**

Variation theorem MO and VB treatment of bonding in molecules – MO theory of homo – and hetero atomic molecules. VSEPR theory – shapes and bonding in molecules of AB_1, AB_2, AB_6, etc. type systems.

UNIT - III: Group Theory-I **(10 Hours)**

Symmetry elements and symmetry operations, point groups, Reducible and irreducible representations, character tables, orthogonality theorem and its consequences, symmetry selection rules for IR Raman and electronic spectral transitions, Systematic procedure for determining symmetries of normal modes of vibration, symmetry applied to MO theory and orbital hybridization.

UNIT - IV: Group Theory-II **(7 Hours)**

Direct product, Direct product representations, Importance of direct product, symmetry selection rules, Projection operators, LCAO approximation, Huckel theory, Symmetry factoring of secular equations, Simplification of Huckel's molecular orbitals, Group theory and Hybridization, HMO calculations.

UNIT - V: Rotational and Vibrational Spectroscopy **(10 Hours)**

Rotational Spectroscopy: Rotational Spectra of diatomic and polyatomic molecules.

Vibrational Spectroscopy: Simple harmonic oscillator and anhormonic oscillator, calculation of force constants from spectra of diatomic molecules Vibration Rotation spectra-PQR branches, interaction of vibration and rotation. Polyatomic molecules, normal modes and normal coordinates. Symmetries of normal modes of vibration and bond assignment for H_2O, CO_2, NH_3, BCl_3, CCl_4, XeF_4, CO stretching frequencies in metal carbonyls. Fundamentals, Overtones, combinations Fermi resonance, polarized Raman Spectra, Laser Raman spectra. Raman selection rule basic principles of Magnetic resonance.

Group frequencies – identification of functional groups, Applications in organic and inorganic chemistry.

Reference Books:

1. Chemical Application of Group Theory, F.A.Cotton, Wiley, 1971.
2. Group Theory – Application to Chemistry, K.V.Raman, TMH,1990.
3. Group Theory ,V.Ramakrishnan, Vishal.
4. Quantum chemistry, Eyrimg,Walter and Kimball.
5. Mathematics for physics and chemistry margenau and Murphy.
6. Introduction to ligand field theory, C.J.Balhauson and H.B.Gray.
7. Introduction to ligand field theory- B.N.Figgis.

Text Books:

1. Physical Chemistry, G. M. Barrow, 4 th Ed., McGraw Hill.
2. Physical Chemistry, P. W. Atkins, 4 th Ed., Oxord.
3. Molecular quantum mechanics, P.W.Atkins, Oxford university press 1983.
4. Quantum mechanics in chemistry, M.W.Haung, W.A.Benjaamen.

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1. https://www.youtube.com/watch?v=IHypiMpMy50
2. https://www.youtube.com/watch?v=hnWu3ey7ifk
3. https://www.youtube.com/watch?v=7jOSbtR8mTs&list=PLyqSpQzTE6M8eGML9tjCEgZjci5USazoW

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	S	M	S	M	L	S	S	S	S
CO 2	M	M	S	S	M	S	M	L	L	M
CO 3	S	S	M	M	L	M	L	M	S	M
CO 4	S	M	S	M	S	S	L	S	S	L
CO 5	M	M	M	S	S	M	S	L	L	M

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Elective	**CHE E302**	**CHE E 302 Macromolecular Chemistry - I**	**3**

Course Objectives:

The main objectives of this course are,

- To provide knowledge about nomenclature of polymer, degree, types, mechanism and kinetics of polymerization.
- To understand the principles of polymer reactivity, stereochemistry of polymerization and various methods of polymerization.
- To know the polymer crystallization, glass transition temperature and Physical and mechanical properties of crystalline and amorphous polymers.
- To improve their analytical skill to analysis and testing of polymer by FT-IR, NMR, XRD, TGA/DTA/DSC.
- To recognize the importance of specialty polymers.

Pre-requisites, if any:

Students should know the UG level fundamental aspects on polymer chemistry.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall the introductory aspects of polymer chemistry. (**K1**)
- **CO2:** Understand the synthesis and characterization methods. (**K2**)
- **CO3:** Apply the knowledge of polymers in diverse areas of basic sciences. (**K3**)
- **CO4:** Analyze and Evaluate the research problems in different areas of polymer chemistry. (**K4** and **K5**).
- **CO5:** Create new concepts to expand the dimensions of polymer chemistry. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Basic Concepts of Polymer Chemistry (9 Hours)

Definition, nomenclature of polymers, functionality of monomers, degree of polymerization. vinylmonomers, initiators, Kinetic chain length, Percentage conversion, chain transfer agents, Mayo's relation, inhibitor, modifiers, and retarders.

Types of polymerization: addition, condensation and copolymerization. Mechanism and kinetics of free radical, cationic and anionic polymerization. Copolymerization: free radical, ionic. Copolycondensation. Types of copolymers, copolymerization reaction, copolymer – comonomer equation, reactivity ratios. Mark Howink equation.

UNIT - II: Polymerization Reactions and Techniques (9 Hours)

Principles of polymer reactivity: Photolytic, photosensitized polymerization. Cyclo, electro-initiated, cross-linking, graft and block copolymerization. Polymer reagents, polymer catalysis.

Stereochemistry of Polymerization: Types of stereoisomerism in polymers, properties of stereoregular polymers. Stereospecific polymerization. Ziegler-Natta polymerization.

Various methods of polymerization: solution, bulk, emulsion and suspension. Electropolymerisation. Comparative accounts. Recycling of polymers.

UNIT - III: Crystal Structure and Properties of Polymers (9 Hours)

Polymer crystallization, factors affecting crystallisability. Morphology of crystalline polymers, effect of crystallisability on the properties of polymers. Glass transition temperature (Tg) and its determination. Dependence of Tg on polymer structure. Melting temperature. Physical and mechanical properties of crystalline and amorphous polymers. Thermal treatment of polymers, Zimmplot.

UNIT - IV: Characterization of Polymers (10 Hours)

Number average, weight average and viscosity average molecular weight of polymers. Molecular weight determination by light scattering, osmotic, centrifuge and viscosity methods. Gel permeation chromatography. Analysis and testing of polymer by FT-IR, NMR, XRD, TGA/DTA/DSC.

UNIT - V: Specialty Polymers (8 Hours)

Polymers in catalysis and drug delivery, Thermosensitive and photo-sensitive polymers, Thermally stable polymers, Biodegradable polymers, Conducting polymers, Fire retardant polymers, polymer electrolytes, Liquid crystalline polymers, Dentrimers, Adhesives, Foams, Fibers.

Text Books:

1. F.W. Billmeyer, Text Book of polymer science Wiley Interscience, 1984.
2. A. Rudin, the elements of polymer science and engineering. An introductory text for engineers and chemists, Academic Press, New York, 1982.
3. M.S. Bhatnagar, A Textbook of Polymers. Vol I. S.Chand & Company Ltd 2004.
4. Bill Meyer. A Text Book of Polymer Chemistry, Singapore: John Wiley & Sons 1994,
5. E.C. Carraher, Introduction to Polymer Chemistry. Taylor & Francis, Inc. 2006.
6. Gowariker & Viswanathan, Polymer Science. Wiley Eastern, 1986.

7. S.P. Mishra, Polymer Chemistry. New Delhi: Wiley Eastern Ltd 1993.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://www.youtube.com/watch?v=54urJPOnaeU&list=PLyqSpQzTE6M_KQ5MqUkoOqAxxOrdvFOMB
2. https://www.youtube.com/playlist?list=PLcCIZORoVQghF126hJD0yU6JZ6ngbOb5a
3. https://www.youtube.com/watch?v=nSAvyQajVzE

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO 5**	**PO 6**	**PO 7**	**PO 8**	**PO 9**	**PO 10**
CO 1	S	S	M	M	S	M	M	S	M	S
CO 2	S	M	S	M	M	M	S	M	M	S
CO 3	M	S	L	S	M	S	M	L	S	M
CO 4	M	S	L	L	M	M	S	M	S	M
CO 5	M	M	S	S	S	M	S	M	M	S

SEMESTER – III

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C601**	**Physical Methods in Chemistry**	**4**

Course Objectives:

The main objectives of this course are

- To provide the deep understanding of electronic and structural changes of metal coordination complexes upon interaction with visible light.
- To understand basic theory & instrumentation involved in the origin of spectroscopy.
- To understand UV, IR, NMR and Mass spectra and their significance in the characterization of organic compounds.
- To illustrate the basic principle of splitting of spectral line of inorganic complexes in the presence of magnetic field upon interaction with electromagnetic radiation.
- To study the role of optical spectroscopy (UV, IR), NMR spectroscopy to understand the structure of organic compounds.
- To learn ESR and their importance in the characterization of radicals.
- To understand basic theory & instrumentation of analytical techniques of characterization

Pre-requisites, if any:

Students should know the the fundamental aspects on spectroscopy and their importance in the characterization of chemical compounds. Basic knowledge on UV-Vis, IR, NMR and Mass spectroscopic techniques will be advantageous.

Course Outcomes:

After completion of this course successfully, the students will be able,

- **CO1:** To interpret absorption bands in the visible, IR and microwave regions, to understand bonding, geometry and reactivity of inorganic coordination complexes. (**K1** – **K4**)
- **CO2:** To understand the basic concept, interpretation and application of electronic spectra of hydrogen and many electron atoms, and to derive angular momentum of many electron atoms and term symbols of atoms. (**K2 – K4**)
- **CO3:**To gain Knowledge on vibrational, ATR and imaging modes to characterize chemical compounds
- **CO4:** To understand the basic theory as well as instrumentation techniques for recording UV, IR, NMR, ESR, MS, XRD, Raman, Mossbauer and Thermal spectra of chemical compounds. (**K2 – K5**)
- **CO5: To** Record and interpret UV, IR, NMR, TGA, DSC, XRD, Raman, Mossbauer, ESR and MS spectra of chemical compounds. (**K3& K4**).
- **CO6:** To understand the nature of functional groups present in chemical compounds using destructive as well as non-destructive spectral techniques. (**K5 & K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Electronic Spectroscopy (PHYSICAL & INORGANIC) (15 Hours)

Spectra of hydrogen and many electron atoms, angular momentum of many electron atoms, term symbols, spectra of many electron atoms- Zeeman effect. Spectra of diatomic molecules, Representation of electronic states through potential energy diagrams-Frank Condon principle.

Intensities of electronic transitions- theoretical treatment of absorption intensities, transition dipole moment integral, oscillator strength, selection rules parity, spin and symmetry considerations, Factors inducing forbidden transitions vibronic and spin orbit coupling, polarization bands.

Spectra of formaldehyde, butadiene and benzene –group theoretical discussion.

Electronic spectra of inorganic complexes – Selection rules (Laporte, orbital and spin selection rules), band intensities, band widths, spectra in solids, spectra of aqueous solutions of d1-d9 ions in Oh and Td environments.

UNIT - II: Spectroscopy (ANALYTICAL) (15 Hours)

Mossbauer spectroscopy – Introduction, principle, instrumentation, recoil energy, Doppler effect, number of MB signals, isomer shift, quadrupole splitting, magnetic hyperfine splitting applications to ^{57}Fe, ^{119}Sn and ^{129}I compounds

Raman Spectroscopy: SERS, SERRS. ATR techniques – UV, IR, Raman. Principle & application of ORD and CD in the identification of complexes.

3D, 4D & 5D NMR imaging techniques

Thermal methods of analysis – TGA, DTA and DSC – Principle and applications.

X-ray diffraction – Bragg equation, space groups and point groups, diffraction methods.

UNIT - III: NMR (ORGANIC) (15 Hours)

Origin of NMR spectrum-Nuclear spin states – NMR active nuclei – Nuclear magnetic moment–Larmor equation – Absorption of energy and Resonance – Population density of nuclear spin states. Saturation phenomena – Relaxation mechanisms, Bloch equation (only significance and derivation not required). Comparison of CW and FT instrument–Chemical shift - Standards in NMR – Shielding and Deshielding – Factors affecting chemical shift – electronegativity, hybridization, hydrogen bonding - anisotropic effect – double, triple bond, aromatic compounds and carbonyl compounds. Spin-spin coupling – splitting origin and rules – factors affecting coupling constant: cis, trans, gem, ortho, meta, para coupling – exchange with deuterium. Vicinity of the proton, Long range coupling, Karplus equation and curve. ^{1}J, ^{2}J, ^{3}J, ^{4}J and ^{5}J coupling in NMR, order of NMR spectrum. Spin systems: Two interacting nuclei: A2, AB, AX, AA'BB', dd, pair of doublet, AB quartet. Three interacting nuclei: AMX, ABX, ABC systems (only pattern is required). Simplification of complex NMR spectra-Lanthanide shift reagents, CIDNP and NOE. Basic principle and applications of VT NMR & MRI.

^{13}C NMR – difficulties in recording ^{13}C NMR: Homo nuclear and heteronuclear coupling. Decoupling technique: SFORD and Off Resonance decoupled spectrum identification of various types of carbon using ^{13}C NMR. APT & DEPT spectrum (DEPT-45, DEPT-90 and DEPT-135).

^{19}F NMR Precessional frequency and heteronuclear coupling. Identification of organofluoro compounds (CF3CO2Et and CF3CH2OH) using NMR. ^{31}P NMR – Chemicalshift and heteronuclear coupling. Identification of organophosphorus compounds suchas (CH3)3P,

(C2H5O)2P=O and Ph3P. P-P bond in NMR.

Basic principles of 2D NMR (COSY, NOSEY, HSQC & HMBC)

UNIT - IV: UV, IR and MS (ORGANIC) & ESR (INORGANIC) (15 Hours)

Electronic absorption-Beer-Lamberts law, Types of electronic excitation. Chromophore and Auxochrome-Bathochromic and Hypsochromic shift. UV-vis spectra of simple organic compounds such as alkenes, phenols, anilines, carbonyl compounds and 1,3-diketones. Woodward and Fieser rule for calculation of λ-max values of dienes and unsaturated ketones.

Infrared Spectra: Identification of functional groups in Organic Compounds, Finger print region. Inter and Intramolecular hydrogen bonding

Origin, basics and bloc diagram of Mass spectrum-Various types of Ionization techniques-Stability of Molecular ions, Meta stable ions. Base peaks and Isotope peaks. Fragmentation patterns of organic molecules such as benzenes, phenyl halides, phenols, benzyl alcohols, benzyl halides, aliphatic alcohols, aliphatic as well as aromatic aldehydes, ketones, acids, esters and amides. Fragmentation patterns of aliphatic/aromatic nitro and amine compounds. Fragmentation patterns of heterocyclic compounds (furan, pyrrole and pyridine only). McLafferty rearrangements of organic molecules.

Structural determination of Organic Compounds using UV, IR, NMR and Mass Spectra.

ESR Spectra of d^1-d^9 Transition Metal Complexes with examples. Interpretation of g in cubic, axial and rhombohedral geometries. Calculation of g values with simple examples. Intensities of '$g_{\parallel}$ and $g_{\perp}$ peaks. Evidence for Metal-Ligand Bond Covalency- Cu(II)- Bis – Salicylaldimine, Bis-Salilcylaldoximato copper(II) $[(NH_3)_5CoO_2CoNH_3)_5]^{5+,}$ Cu(II)-diethyldithiophosphinate, Vanadyldithiophsphinate, Copper(II) tetraphenylporphyrin, Co(II)-phthalocyanine, $K_2[IrCl_6]$. Interpretation of 'g' and 'A' values from esr spectral data in- i) MnF_6^{4-}, ii) CoF_6^{4-}, and CrF_6^{3-}.

Contemporary Issues:

Expert lectures, YouTubes Videos, Animations, NPTEL, MOOC videos, online seminars – webinars for strengthening the subject matters.

Text Books:

1. Basic Principles of Spectroscopy, R. Chang, McGraw Hill
2. Fundamentals of Molecular Spectroscopy, Fourth Edition, Colin N. BANWELL and Elaine M. McCASH
3. Kemp, W. (2016); Organic Spectroscopy, 3rd Edition, Palgrave.
4. Kalsi, P. S (2016); Spectroscopy of Organic Compounds, 7th Edition, New Age International.
5. Silverstein, R. M, Webster, F. X, Kiemble, D. J, Bryce, D. L (2015); Spectrometric Identification of Organic Compounds, 8th Edition, Wiley.
6. Jag Mohan (2016); Organic Spectroscopy Principles & Applications, 3rd Edition, Narosa Publishing House.
7. Pavia, L, Lapman, G. M, Kriz, S, Vyvyan, J.-R (2015); Introduction to Spectroscopy, Cengage Learning, ISBN 13: 978-81-315-2916-4.
8. Physical Methods in Chemistry, R. S. Drago, W.B. Saunders Co., 1977.
9. E. Huheey, E. A. Keiter, R. L. Keiter, O. K. Medhi; Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed. Pearson Education, 2006.

10. Principles of Instrumental Analysis – Douglas A. Skoog, F. Holler, Stanley Crouch, 7thEdn Brooks/Cole publish; 7th edition, 2017

Reference Books:

1. Structural Methods in Inorganic Chemistry, E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, ELBS.
2. Physical Methods For Chemists, Russell S. Drago Second Edition, 2016.
3. Huheey, J.E. - Inorganic Chemistry, 4th Edition, Harper and Row.
4. Lambert, J. B, Shurvell, H. F, Lightner, D. A, Graham Cooks, R (1998); Organic Structural Spectroscopy, Prentice Hall, ISBN: 0-13-258690-8.
5. Macomber, R. S (1998); A complete introduction to Modern NMR Spectroscopy, John Wiley, ISBN: 0-471-15736-8.
6. Willard, H.H.; Merritt, L.L. Jr.; Dean, J.A.; Settle, F.A. Jr., CBS Publishers & Distributors; 7th edition (2004).

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://nptel.ac.in/content/storage2/courses/102103044/pdf/mod2.pdf
2. https://www.slideshare.net/LOKESHPANIGRAHI/spectroscopy-134933430
3. https://www.slideshare.net/guest824336/introduction-to-spectroscopy
4. http://web.iyte.edu.tr/~serifeyalcin/lectures/chem305/cn_1.pdf
5. https://www.youtube.com/watch?v=qtpVfccYEHE&t=98s
   http://www.digimat.in/nptel/courses/video/104106122/L54.html
6. https://pubs.rsc.org/en/content/articlelanding/2018/cs/c6cs00565a
7. https://chem.libretexts.org/Bookshelves/Physical_and_Theoretical_Chemistry_Textbook_Maps/Supplemental_Modules_(Physical_and_Theoretical_Chemistry)/Spectroscopy/Magnetic_Resonance_Spectroscopies/Electron_Paramagnetic_Resonance/EPR%3A_Application

Course Designed By:

Prof. A. K. Mohanakrishnan, Dr. K. Parthasarathy, Dr. A. Murugadoss, Dr. T.M. Sridhar, Dr. K. Venkaachalam and Dr. Deepa P Nambiar

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	M	S	S	M	M	S	M	M	L	L
CO 2	S	M	S	S	M	M	S	M	L	L
CO 3	S	M	S	M	L	M	S	L	L	L
CO 4	M	S	S	S	L	S	M	L	L	L
CO 5	S	S	S	M	L	L	S	L	L	L
CO 6	S	M	S	M	L	M	S	L	L	L

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Elective	**CHE E601**	**Biological Chemistry**	**3**

Course Objectives:

The main objectives of this course are,

- To understand the function of carbohydrates in biological chemistry, determination of ring size and study of starch and cellulose.
- To understand the significances of amino acids, proteins nucleic acids in biological system.
- To illustrate the importance of the various elements in the biological system and to gain more insights into the binding of metal complexes with biomacrmolecules and transport and storage mechanism involved in the metaloenzymes.
- To understand the role of heavy metals in the human body- therapeutic and toxicity levels.

Pre-requisites, if any:

Student able to understand the role of bio-organic compounds. Students should know the fundamental aspects on biological system, mechanism, kinetics and analytical tools.

Course Outcomes:

After completion of this course successfully, the students will be able,

- **CO1:** To discuss the structure and functions of carbohydrates, lipids, membranes, amino acids, proteins, antibiotics and vitamins. (**K1 - K5**)
- **CO2:** To explain the biological importance of RNA and DNA. (**K2 - K4**)
- **CO3:** To understand the key functions of metal ions such as Fe, Co, Ni Zn and Cu in living systems, particularly in transport (energy and O_2), storage, electron- and proton transfer, hydrolysis, etc. which are taking place at the active sites of metalloproteins and enzymes. (**K1-K4**)
- **CO4:** To explain the toxicity of metals and their effects in the biological system. (**K1- K4**)
- **CO5:** To evaluate toxicity of drugs used in cancer and radiodiagnosis. (**K5& K6**).

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Bio-organic Chemistry **(11 Hours)**

Carbohydrates: Pyranose and furanose forms of aldohexose and ketohexose – methods used for the determination of ring size - conformation of aldohexopyranose – structure and synthesis of lactose and sucrose. A brief study of starch and cellulose.

Lipids and Membranes: Molecular structure of lipids. Fatty Acids, TriglyceridesTypesof membrane lipids.

Amino acids and Proteins: Amino acids and Protein structure, Analysis ofN-terminal and C-terminals in a polypeptide. Sanger method, Edman degradation and Enzymaticanalysis.Primary, secondary and tertiary structure of proteins. Structure of collagen, myoglobin and haemoglobin.

Nucleic acids: Chemistry of nucleic acids, nucleosides and nucleotides – Structure RNA and DNA and their biological importance.

Biomolecules: Antibiotics and vitamins: A detailed study of structure, and stereochemistry of penicillin, cephalosporin. Chemistry and physiological action of ascorbic acid, thiamin, riboflavin and pyridoxine – Elementary aspect of vitamin A, E, K and $B_{12.}$

UNIT-II: Bioinorganic Chemistry (12 Hours)

Essential and trace metal ions: Enzymes - Nomenclature and classification – Coenzymes - Vitamin B_{12}, carboxypeptidase and Superoxide dismutase – Heme-enzyme - Peroxidase and catalases. Oxygen carriers: Hemeproteins - Hemoglobin, myoglobin - Structure Oxygenation and stereochemistry - Bohr effect. Non-heme oxygen carriers - Hemerythrin and hemocyanin. Nitrogen fixation: Introduction, types of nitrogen fixing micro organisms. Nitrogenase enzyme - Metal clusters in nitrogenase - redox property - Dinitrogen complexes - transition metal complexes of dinitrogen - nitrogen fixation via nitride formation and reduction of dinitrogen to ammonia. Biological redox systems: Cytochromes -Classification, cytochrome a, b and c. Cytochrome P-450. Transport of electrons: Iron-Sulphur Proteins: Rubredoxins and Ferredoxins, Structural and Spectral features of Iron-Sulphur Proteins. Photosynthesis and chlorophyll's.

UNIT-III: Biophysical Chemistry (11 Hours)

Thermodynamics and biology – Basic concepts of structure and functionality – membranes – structure, function transport properties, aspects of electrochemical phenomena – active transport, ionophores, biological energy storage systems – stepwise mechanism of photosynthesis versus potential. Enzymes - Nomenclature and classification, chemical kinetics, the free energy of activation and the effects of catalysts, kinetics of enzyme catalyzed reactions – Michaelis - Menten equation - Effect of pH, temperature on enzyme reactions, Factors contributing to the catalytic efficiency of enzymes. Membranes - Phase Equilibria, Donnan effect, Donnan Potential, Phase transition in Lipid bilayers, Free energy determination for ATP hydrolysis from sodium-potassium pump, Allosteric effects – Monod-Wyman-Changeux Theory, Assigning of Statistical weights for Helix-Coil transition in proteins, Study by spectroscopic methods.

UNIT- IV: Bioanalytical Chemistry (11 Hours)

Essentials of trace elements and chemical toxicology: Trace elements in biological system. Metal ion toxicity - classes of toxic metal compounds – detoxification. Metals in medicine: Anti arthritis drugs – Au and Cu in rheumatoid arthritis – Li in psychiatry – Pt, Au and metallocenes in anti cancer drugs- metals in radiodiagnosis, radio therapy and magnetic resonance imaging. Transport and storage of metals: Mechanism – Fe, Cu, Zn and V storage and transport – metallothioeins. Molecular mechanism of iron transport across the membrane – sodium and potassium ion pumps. Pollution studies – Effluent and water treatment

Text/Reference Books:

1. Zubay, G, L. (1997); Biochemistry,4th edition, Brown (William C.) Co
2. Nelson, D, L Lehninger, A, L CoxM, M.(2008); Principles of Biochemistry, 5th Edition, New York: W.H. Freeman.
3. John McMurray, (2008); Organic Chemistry, 8th edition, Brooks/Cole.
4. Finar, I. L. Vol 2 (2018); Organic Chemistry: Stereochemistry and the Chemistry of Natural product, IIIrd Ed, Pearson

5. Williams D. R. (1976); Introduction to Bioinorganic Chemistry, Thomas, ISBN-13 : 978-0398034221.
6. Kaim, W,Schwederski, B,Klein, A. (2013);Bioinorganic chemistry: Inorganic Elements in the chemistry of life, 2nd edition, Wiley.
7. Das Asim K. (2007); Bioinorganic Chemistry, 1st edition, Books and Allied (P) Limited.
8. Mugherjee G. N,Arabinda D, (1993); Elements of Bioinorganic Chemistry, 4th Edition, U. N. Dhur& Sons Pvt. Ltd.
9. Satake M. MidoY. (1996); Bioinorganic Chemistry, ISBN 81-7141-301-1, Discovery Publishing House, New Delhi.
10. Eichorn, G, (1973); Inorganic Bio-Chemistry Vol. I and II, IV Ed, Elsevier.
11. Zhimin, T, (2008); Analysis of Cytotoxicity of Anticancer Drugs, VDM Verlag Dr. Mueller E.K.ISBN: 9783639063486, 3639063481.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]:

1. https://www.youtube.com/watch?v=iuW3nk5EADg
2. https://www.youtube.com/watch?v=aeC7M9PDjQw
3. https://www.youtube.com/watch?v=DhwAp6yQHQI
4. https://www.youtube.com/watch?v=ZqoX2W1N6l0
5. https://www.youtube.com/watch?v=lsNalwRnaq0&list=PLbMVogVj5nJSHhL_cMKfzLv556ddrIT90
6. https://www.youtube.com/watch?v=pXztk04J7u0&list=PLFW6lRTa1g83-gUOcT3ay875UG3a9Mu11

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO 5**	**PO 6**	**PO 7**	**PO 8**	**PO 9**	**PO 10**
CO 1	L	M	L	M	M	M	M	M	L	M
CO 2	L	M	L	S	L	M	L	M	M	M
CO 3	L	L	M	S	L	L	M	L	L	M
CO 4	L	L	L	M	L	M	L	M	L	L
CO 5	M	L	M	M	L	L	M	L	L	S

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C309**	**Advanced Materials for Catalysis and Drug Delivery Applications**	**4**

Course Objectives:

The main objectives of this course are,

- To provide the complete fundamentals of catalysis.
- To understand the chemistry of catalyst synthesis.
- To understand various reactions of homogenous catalysis.
- To understand enzyme catalysis and phase transfer catalysis.
- To get complete knowledge on chiral catalysts and asymmetric synthesis.
- To get clarity on cracking of heavy oil, naphtha reforming and other refinery processes.

Pre-requisites, if any:

Students should know the fundamental aspects on catalysis and drug action mechanism.

Course Outcomes:

After completion of this course successfully, the students will be able,

- **CO1:** To get scientific maturity in catalysis. (**K1 - K5**)
- **CO2:** To understand the catalytic processes in chemical industries or refineries. (**K2 - K4**)
- **CO3:** To apply the knowledge of catalyst in controlling reaction kinetics. (**K1-K4**)
- **CO4:** To know recent developments in drug delivery research progress. (**K1- K4**)
- **CO5:** To create research problems in drug delivery strategies. (**K5 & K6**).

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Fundamentals of catalysis **(12 Hours)**

Industrial applications of catalysis, classification of catalysis-homogeneous and heterogeneous catalysis, catalyst preparation-precipitation, coprecipitation, impregnation, ion exchange, hydrothermal synthesis, synthesis osupported catalysts, zeolites, AlPOs and mesoporous materials characterization of catalysts-Textural characterization by BET,XRD, FTIR, DRS UV Vis, XPS, SEM and TEM, Thermal programmed methods of characterization-Temperature programmed desorption, reduction, oxidation, TGA, SEM. Kinetics and mechanisms of catalysis, Contact time, weight hourly space velocity, time on stream, Turn over number and turn over frequency.

UNIT-II: Industrial applications of catalysts **(12 Hours)**

Applications of homogeneous and heterogeneous catalysis- Application of homogeneous catalysis-carbonylation of alcohols, reduction of organic compounds with molecular hydrogen and hydride, application of telomerisation and dimerization to the synthesis of fine chemicals, oligomerization of olefins, coordination polymerization of mono olefins, Chirality and biological activity, catalytic asymmetric synthesis, enzymatic transformation, phase transfer catalysis, Electrocatalysis, synyhetic petrol by catalytic cracking of heavy oil, catalytic cracking of naphtha, catalytic naphtha reforming, Hydrodesuphurization, hydrodenitrogenation,

hydrodeoxygenation.

UNIT-III: Functionalization of Nanomaterials - Dendrimers and Carbon nanotubes (12 Hours)

General methods for the Synthesis of Nanomaterials – Chemical approach Manipulation of Nanoparticles - Nanofabrication. Functionalization of Nanomaterials- Carbon nanotubes (CNT) – Dendrimers - Metal Nanoparticles and Core - Shell nanocomposites. CNT - Functionalization of CNT-caps, open ends and side wall, covalent and non-covalent attachment of functional groups, composite materials with carbon nanotubes, Elementary Introduction to - carbon onions and related materials, nanodiamonds, nanofilms nanowires, nanofluids, quantum dots, nanoshells for catalysis, sensors, medicine, biodevice fabrication applications. Graphene – Basic concepts, structures and applications of graphene based materials.

UNIT- IV: Drug delivery (12 Hours)

Fundamentals of drug delivery system - Use of polymers in drug delivery - Pharmacokinetic and Pharmacodynamics basis of drug delivery - Various types of drug delivery systems. Biochemical and molecular biology approaches to controlled, sustained and targeted drug delivery systems- Proteins and peptide drug delivery. Drug targeting to particular organs - Drug delivery to respiratory system, drug delivery to the brain and Drug delivery to eye. Drug delivery using surfactants, dendrimers, nanoparticles and carbon nanotubes-solubility of drugs.

UNIT- V: Advanced Characterizations Techniques (12 Hours)

Characterization of catalysts: Surface area by BET method. Determination of pore volume and pore size distribution by BJH method - Pore size and specificity of catalysts. Surface acidity of catalysts - Determination of surface acidity by indicator, IR spectroscopic and TPD methods. Thermal analysis: TGA, DTA, DSC - Basic principles – Instrumentation – applications. Testing the purity and characterizations of various materials. Principles, Instrumentations, measurements and analysis for surface characterization by microscopic techniques and Electron imaging techniques - Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), X-Ray Diffraction – X-Ray Photoelectron spectroscopy - Atomic Force Microscopy (AFM) studies.

Text/Reference Books:

1) B. Viswanathan, Catalysis selected application, Narosa, 2009.
2) J. M. Thomas and W. J. Thomas, Principles and Practice of Heterogeneous Catalysis, VCHPublishers Inc., New York, USA., 2008.
3) Industrial Catalysis Jens Hagen, WILEY-VCH Verlag GmbH& Co. Weinheim, Germany (2006).
4) D. K. Chakrabarty and B. Viswanathan, Heterogeneous Catalysis, New Age, 2008.
5) The Chemistry of catalytic conversions, Herman Pine, Academic Press, New Delhi (1981).
6) ERTL, G. -- WEITKAMP, J. -- KNOZINGER, H. Handbook of heterogeneous catalysis . Weinheim: Wiley-VCH, 1997.
7) B. Viswanathan, S.Kannan and R.C.Deka, Catalysis and surfaces characterisation techniques
8) Polymers and Polymer Composites in Construction L.C. Holleway,1990.

9) Carbon Materials and Nanotechnology. Anke Krueger, 2010.
10) NANO - The Essentials, Understanding Nanoscience and Nanotechnology. T.Pradeep, Seventh Reprint, 2012.
11) R.A. Sheldon, Chirotechnology. Industrial applications of optically active compound, Marcel Tekker, Inc.,New york 1993.
12) Julion R.H. Rose, Heterogeneous catalysis and applications, Elsevier, 2012.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]:

1) https://www.youtube.com/playlist?list=PLbMVogVj5nJQVyjZ-lEYm8Sp1jSynW9MD
2) https://www.youtube.com/watch?v=u0_CEbn7tio&list=PLgMDNELGJ1Cb10Fl8jYh4JnAV3NcQ1wVu
3) https://www.youtube.com/watch?v=8YflxVwm6cE

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	M	S	M	S	L	S	L	S	S
CO 2	S	L	M	S	M	S	L	M	M	M
CO 3	M	S	L	L	L	M	M		M	S
CO 4	M	M	S	M	S	S	M	M	L	S
CO 5	S	S	M	L	M	M	S	L	S	M

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Elective	**CHE E602**	**Photochemistry and Nanomaterials**	**3**

Course Objectives:

The main objectives of this course are,

- To recall and understand the fundamental concepts of photochemistry and principles of fluorescence spectroscopy for investigating photophysical phenomena.
- To illustrate different photochemical reactions of coordination and organometallic complexes.
- To gain knowledge on the faster reaction kinetics studies.
- To know various techniques employed for the capturing of reactive transient species in a reaction.
- To have basic understanding of size dependent properties in nanoscale materials.
- To describe nano systems, their properties, synthetic methods, structure and applications.
- To make them to learn different analytical techniques of microscopy to characterize nano materials.

Pre-requisites, if any:

Students are expected to have basic idea about photochemistry, various reactive intermediates generated during chemical reactions and organometallic complexes. They should know the basic quantum chemistry to understand Nanomaterials and their properties.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Distinguish different photochemical processes such as fluorescence, phosphorescence, non-radiative decay, etc. (**K2-K3**)
- **CO2:** Understand the effect of environments like solvents, neighboring molecules on photochemical decay processes of molecules. (**K1-K2**)
- **CO3:** Quantify the parameter of decay kinetics after photo-excitation. (**K3-K4**).
- **CO4:** Compare photolytic techniques induced by light and ionizing radiation. (**K3-K5**)
- **CO5:** Elucidate various methods of synthesis, properties and applications of nano materials. (**K5-K6**)
- **CO6:** Illustrates the basic components of an artificial photosynthetic system assembled in different ways. (**K3-K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT – I: Photophysical Phenomena **(15 Hours)**

Fundamentals of photochemistry – photochemical laws – emission of radiations – types of photophysical pathways – delayed fluorescence – basic instrumentation of steady-state and time-resolved fluorometer – fluorescence emission, solvent and environmental effects, red-edge effects, effects of intermolecular photophysical processes on emission – static and dynamic quenching, Stern-Volmer kinetics – emission anisotropy – electron transfer probes – energy transfer in multiple acceptors.

UNIT – II: Photochemistry of Inorganic complexes **(15 Hours)**

Inorganic photochemistry – photoredox and isomerization process – Photo substitution reactions– photosensitization reactions – photochemistry in energy conversion, application of metal complexes in solar energy conversion; organometallic photochemistry –photochemical reactions in metal carbonyls; Photochemical techniques – flash photolysis – lasers in photochemistry; radiation chemistry – primary processes – track effects – dosimetry – pulse radiolysis.

UNIT – III: Nanoscale Materials **(15 Hours)**

Definition of a nano system - classification of nanoscale materials - dimensionality and size dependent phenomena – Quantum effect – Nanoscale effects in size dependent variation in mechanical, physical and chemical, magnetic, electronic transport, reactivity – Methods of preparation. Top to down and Bottom up approach – Mechanical, Physical and Chemical methods; Structural characterization; different types of electronic spectroscopy – Elemental composition; Electron spectroscopies – Morphological characterization – Electron microscopy; SEM – TEM – Force microscopies; Application of nanoscale materials.

Text Books:

1. Physical Chemistry: D.W. Ball

2. Flash photolysis and pulse radiolysis- R.V. Bensasson, E. J. Land and T. G. Truscott, Pergamon Press
3. Fundamentals of photochemistry- K. K. Rohtagi and Mukherjee, New Age International (P) Ltd. Publishers
4. The exploration of Supramolecular systems and Nanostructures by photochemical techniques, Volume 78, Paola Ceroni editor, Springer
5. Nanomaterials: An introduction to synthesis, properties and application, Dieter Vollath, WILE-VCH, 2008
6. Adamson, A. W-, and Fleischauer, P. D., (Editors) "Concepts of Inorganic Photochemistry," Wiley-Interscience, New York, 1975.

Reference Books:

1. Theoretical Chemistry by S. Glasston
2. Modern Aspects of Inorganic Chemistry-H.J. Emeleus and A.G. Sharpe
3. Fundamentals of Radiation Chemistry- A. Mozumder, Academia Press
4. Nanostructures & Nanomaterials: Synthesis, Properties &Applications" G. Cao, Imperial College Press, 2004
5. Balzani, V., and Carassiti, V. "Photochemistry of Coordination Compounds," Academic Press, New York, 1970.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://www.youtube.com/watch?v=hIHNUVBvVkU
2. H. Hennig, D. Rehorek, R.D. Archer. Photocatalytic systems with light-sensitive coordination compounds and possibilities of their spectroscopic sensitization—an overview. Coordination Chemistry Reviews 1985, 61 , 1-53
3. https://nptel.ac.in/courses/104/103/104103069/
4. https://nptel.ac.in/courses/104/105/104105038/
5. https://onlinecourses.nptel.ac.in/noc21_cy04/preview
6. https://nptel.ac.in/courses/104/106/104106077/

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO 5**	**PO 6**	**PO 7**	**PO 8**	**PO 9**	**PO 10**
CO 1	M	M	S	S	M	M	S	L	L	L
CO 2	S	L	M	S	S	M	S	L	L	L
CO 3	S	S	M	S	S	S	M	L	L	L
CO 4	S	S	S	S	S	S	S	L	M	L
CO 5	S	S	L	M	M	L	S	L	S	L
CO 6	S	S	M	S	S	S	M	L	L	L

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C304**	**Physical Chemistry Practical- II**	**3**

Course Objectives:

The main objectives of this course are,

- To provide experimental knowledge on kinetics by determining rate constant, energy of activation, order of the reaction through acid-base and conductometric titrations.
- To illustrate the kinetics of ionic reactions, enzyme catalyzed reactions, salt and solvent effects on reaction rate constant.
- To give experimental knowledge on partition method, partial molal volvume, phase diagram, and surface tension experiments.
- To demonstrate experiments on stability constant of a complex, heat of combustion, heat of solution of a salt, heat of neutralization of a polybasic acid.
- To correlate the experimental knowledge in kinetics and thermodynamic experiments for applying in the research problems of chemistry.

Pre-requisites, if any:

Students should know the UG level fundamentals of physical chemistry practicals like solution preparation, normality, molarity, dilution of solution, kinetic and thermodynamic concepts.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **O1:** Recall the basics and practices of physical chemistry practicals. (**K1**)
- **O2:** Understand the experimental aspects of kinetic and thermodynamic problems. (**K2**)
- **O3:** Apply the knowledge of experimental physical chemistry to existing and emerging problems in basic science. (**K3**)
- **O4:** Analyze and Evaluate the research problems with reference to these experiments in different areas of physical chemistry. (**K4** and **K5**)
- **O5:** Create new concepts to the growth of the experimental physical chemistry with reference to these experiments. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

Experiments **(135 Hours)**

1. Determination of the rate constant and energy of activation of hydrolysis of ethyl acetate.
2. Study of the kinetics of the reaction between acetone and iodine in acetic medium by half life method and determination of the order with respect to iodine and acetone.
3. Study of the saponification of ethyl acetate by sodium hydroxide by conductometry and evaluate the rate constant.
4. Study of the primary salt effect on the kinetics of ionic reactions and test the Bronsted relationship, (iodide ion is oxidized by persulphate ion).
5. Study of the kinetics of enzyme catalyzed reactions.
6. Study of the salt and the solvent effect on the rate of alkaline hydrolysis of crystal violet.

7. Study of the complex formation between copper sulphate and ammonia solution by partition method.
8. Determination the molecular weight of a polymer by viscosity method.
9. Determination of the partial molal volume of glycine/methanol/formic acid/sulphuric acid by graphical method and determining the densities of the solutions of different compositions.
10. Construction of the phase diagram of the three components of partially immiscible liquid systems (chloroform – acetic acid – water).
11. To study the surface tension – concentration relationship for solutions (Gibb's equation).
12. To construct a chemical actinometry and determination of the quantum yield and calibration of lamp intensity.
13. Determination of stability constant of a complex by spectrophotometery
14. Determine heat of combustion of a substance by bomb calorimetry.
15. Determine integral and differential heat of solution of a salt.
16. Determine heat of neutralization of a polybasic acid – citric acid.

Text Books:

1. B.P. Levitt Findlays Practical Physical Chemistry (9th.ed.) Longman Group Ltd. 1973.
2. Experimental Physical Chemistry, GP Mathews, Oxford, 1985.
3. Experimental Physical Chemistry, VD Athawale P Mathur, 2001.

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	S	S	M	S	S	L	M	M	M
CO 2	M	M	M	L	L	S	M	M	M	L
CO 3	S	S	M	L	S	L	S	S	L	S
CO 4	S	M	M	M	S	L	M	L	S	M
CO 5	M	S	S	S	L	M	L	S	M	M

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C305**	**Physical Chemistry Practical- III**	**3**

Course Objectives:

The main objectives of this course are

- To provide knowledge on conductometric experiments for studying mixture of acids and relative strength of acids.
- To illustrate the applications of potentiometric experiments for the determination of electrode potentials, activity coefficient, dissociation constant, complex formation constant and formal redox potential.
- To give experimental knowledge in colorimetric determination of pK value of an acid-base indicator.

- To develop skill for interpretation and data analysis on IR, NMR, UV-Vis and powder XRD results.
- To apply the experimental knowledge of conductometric, potentiometric and colorimetric experiments to the different research problems in chemistry.

Pre-requisites, if any:

Students should know the UG level fundamentals of physical chemistry practicals like solution preparation, normality, molarity, solution dilution, conductometric, potentiometric and colorimetric experiments.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall the basics and practices of physical chemistry practicals. (**K1**)
- **CO2:** Understand the experimental aspects of conductometry, potentiometry and colorimetry (**K2**)
- **CO3:** Apply the knowledge of experimental physical chemistry to existing and emerging problem in basic sciencess. (**K3**)
- **CO4:** Analyze and Evaluate the research problems with reference to these experiments in different areas of physical chemistry. (**K4** and **K5**)
- **CO5:** Create new concepts for elaborating the experimental physical chemistry with reference to these experiments. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

Experiments **(135 Hours)**

1. Conductometric titrations of a mixture of HCl and acetic acid, and copper sulphate and sodium hydroxide.
2. Comparision the relative strength of acetic acid and monochloro acetic acid by conductance method.
3. Determination of the electrode potentials of Ag electrodes in 0.1 M and 0.001 M solutions at 298 K and find standard potentials for these electrodes and test the validity of Nernst equation.
4. Determination of the activity coefficient of an electrolyte at different molalities by EMF measurements.
5. Determination of the dissociation constant of acetic acid and a dibasic acid by titrating it with sodium hydroxide using quinhydrone as an indicator electrode and calomel as a reference electrode.
6. Determination thepKa value of an acid base indicator (methyl red) by colorimetry.
7. Determination of the formation constant of silver ammonia complex and stoichiometry of the complex potentiometrically.
8. IR, 5NMR, 5UV-Vis spectra and 2 X-ray diffraction data will also be supplied for interpretation and calculation of data. (Note: The list of typical spectra to be given is under consideration and will be made available in due course).
9. Determination of the formal redox potential of Fe^{2+}/Fe^{3+} by potentiometry.

Text Books

1. B.P. Levitt Findlays Practical Physical Chemistry (9th.ed.) Longman Group Ltd. 1973.
2. Experimental Physical Chemistry, GP Mathews, Oxford, 1985.
3. Experimental Physical Chemistry, VD Athawale P Mathur, 2001.

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	M	L	M	M	S	S	L	M	M
CO 2	M	M	L	L	M	M	S	M	L	L
CO 3	S	S	M	S	L	S	S	M	S	L
CO 4	M	L	S	S	M	S	M	M	L	M
CO 5	M	L	M	L	M	S	S	S	M	M

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Supportive	**UOMS117**	**Chemistry Databases – SciFinder, Mandeleef, Scopus, Web of Science and Google Scholar**	**2**

Course Objectives:

The main objectives of this course are,

- To analyze, categorize and refine the Scifinder database based on the different components of research article.
- To learn Mandeleef for the management of references and Scopus for analysis of research database.
- To train Web of Science and Google Scholar database to analyze, categorize and refine the different components of research articles.
- To know the systematic procedure for collecting literature in the identified research area using scientific resources.
- To develop skill for creating a new synthetic scheme or protocol based on the literature search.

Pre-requisites, if any:

Students should know the components of journal and research article.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall different components of research article and literature search. (**K1**)
- **CO2:** Understand the importance of SciFinder, Mandeleef, Scopus, Web of Science and Google Scholar in scientific data collection. (**K2**)
- **CO3:** Apply the systematic procedure for collecting literature in the identified research area using different scientific resources. (**K3**)
- **CO4:** Analyze and Evaluate research problems using different scientific data collection resources. (**K4** and **K5**).

- **CO5:** Create new research problems using the systematic collection of literatures. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: SciFinder Database **(6 Hours)**

Components of SciFinder, Analyzing, Categorizing and Refining the Scifinder database based on Research topic, Author name, Company name, Molecular formula, Molecular structure, Chemical reaction, Journals, Patents, Physical Properties. Importance of Scifinder database in planning a research problem.

UNIT - II: Mandeleef **(6 Hours)**

Mandeleef Reference Manager – Application; Reference file - Collection, Insertion, Library organization, Notebook; Citation database - analyze- visualize - research. h- Index, h-graph Cite Score, SJR (SCImago Journal Rank) and SNIP (Source Normalized Impact Paper). ORCHID, Citable documents, Citations, Self Citations - Document types- Alternative Metrics. Overview, citations, Scholarly commentary, Citation Benchmarking, Advanced Search,

UNIT - III: Scopus **(6 Hours)**

Components of Scopus, Analyzing, Categorizing and Refining the Scopus database based on different options. Importance of Scopus database in planning a research problem. Proximity characters in Scopus.

UNIT - IV: Web of Science **(6 Hours)**

Web of Science – History, Components of Web of Science, Analyzing, Categorizing and Refining the Web of Science database based on different options. Importance of Web of Science database in planning a research problem.

UNIT-V: Google Scholar **(6 Hours)**

Google Scholar – History, Features and specifications, Ranking algorithm, Groups and access to literature - Limitations and citations, Search engine. Citations, H-index and i10 index – Keywords search - Steps to create google scholar ID and Addition/Removal of articles – Profile updates – My library- Metrics- Alerts -Merits and Demerits of Google Scholar ID.

References:

1. https://www.cas.org/support/training/scifinder
2. https://www.cas.org/sites/default/files/documents/scifinder_search_references_workbook.pdf
3. https://www.mendeley.com/reference-management/mendeley-cite
4. https://www.elsevier.com/solutions/scopus
5. https://clarivate.libguides.com/webofscienceplatform/alldb

6. Jensenius, F., Htun, M., Samuels, D., Singer, D., Lawrence, A., &Chwe, M. (2018). "The Benefits and Pitfalls of Google Scholar" PS: Political Science & Politics, 51(4), 820-824.

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	M	S	L	M	S	S	S	M	M	L
CO 2	S	M	S	L	L	M	S	M	L	S
CO 3	M	S	L	M	S	M	S	M	M	S
CO 4	S	S	M	S	M	S	S	L	S	M
CO 5	S	M	S	M	S	S	M	M	M	L

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Internship	**UOM1001**	**Internship**	**2**

Course Objectives:

The main objectives of this course are,

- To give industrial research exposure in physical chemistry.
- To learn industrial protocol for the execution of a research problem.
- To apply knowledge to develop new synthetic/ process route based on the literature search.
- To execute experiments, and to collect & analyze the data.
- To prepare the research report based on the obtained results.

Pre-requisites, if any:

Students should select any research industries or any other academic/research institutions and have to give a research proposal on the area of research work.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall the basics of chemistry to execute an industrial research. (**K1**)
- **CO2:** Understand the methodologies for collecting literature search. (**K2**)
- **CO3:** Apply the knowledge for systematic execution of a research work. (**K3**)
- **CO4:** Analyze and Evaluate the research data with reference to literature. (**K4** and **K5**)
- **CO5:** Create new research report based on the outcome of research work. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

Detailed Syllabus **(4 Weeks)**

Students are allowed to select any Chemistry Industries or any or any other academic/research institutions to do internship program in any specific field of interest.

Once the selection of Industry/Research Laboratory is finalized, the student has to work at there. Students will be periodically assessed for their project work by the individual Industry/Research Laboratory.

The final submission of the internship project report i.e. small thesis, presentation, and comprehensive viva carries 100% marks.

Note:

1. Student should submit 3 copies of the final internship research project report in hard binding format with all declarations and signatures.
2. For referencing any ACS journal pattern should be followed.

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	**PO 2**	**PO 3**	**PO 4**	**PO 5**	**PO 6**	**PO 7**	**PO 8**	**PO 9**	**PO 10**
CO 1	M	M	S	M	M	S	M	M	S	S
CO 2	S	S	M	L	S	M	L	M	L	M
CO 3	S	M	S	M	S	L	S	S	L	S
CO 4	M	S	M	L	M	M	M	M	S	L
CO 5	S	M	M	S	M	S	L	S	L	M

SEMESTER – IV

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C306**	**Advanced Thermodynamics & Kinetics of Chemical Reactions and Electrochemistry**	**4**

Course Objectives:

The main objectives of this course are,

- To provide fundamentals of statistical thermodynamics and partition functions, and their applications to heat capacities of ideal gases and solids.
- To learn theories, laws, effects, principles and applications of irreversible thermodynamics.
- To apply the concepts of kinetics for complex reactions, factors of reaction rate and homogeneous catalysis.
- To understand the mechanisms of electrode reactions and H_2& O_2 evolution reactions, and corrosion studies.
- To develop the ability to do some independent research problems and use some experimental resources at the end of the course.

Pre-requisites, if any:

Students should know the fundamental aspects of fundamentals of thermodynamics, chemical kinetics and electrochemistry s along with problems solving.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall basics of statistical and irreversible thermodynamics, kinetics of complex and electrode reactions. **(K1)**
- **CO2:** Understand the importance of statistical and irreversible thermodynamics, kinetics of complex and electrode reactions in different areas of chemistry. (**K2**)
- **CO3:** Apply the knowledge of statistical and irreversible thermodynamics, kinetics of complex and electrode reactions to different research problems. (**K3**)
- **CO4:** Analyze and Evaluate the different research problems in statistical and irreversible thermodynamics, kinetics of complex and electrode reactions. (**K4** and **K5**).
- **CO5:** Create new concepts to expand the dimensions of statistical and irreversible thermodynamics, kinetics of complex and electrode reactions. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Statistical Thermodynamics-I **(15 Hours)**

Objectives of statistical thermodynamics – Concept of thermodynamic and mathematical probalities – distribution of distinguishable and indistinguishable particles. Types of Statistics- Thermodynamic probability (W) and Derivations of Maxwell-Boltzmann, Fermi-Dirac and Bose – Einstein statistics, Ideas of microstates and macrostates - Lagrange's undetermined multipliers – Stirling's approximations - comparison and applications of statistics. Modes of contribution to energy; ortho and para hydrogen.

UNIT - II: Statistical Thermodynamics-II (12 Hours)

Partition function – evolution of translational, vibrational and rotational partition functions, thermodynamic functions in terms of partition functions – calculation of equilibrium constants from partition functions (isotope exchange and dissociation of diatomic molecules) – application of partition functions to heat capacities of ideal gases – heat capacities of solids (Einstein and Debye models)

UNIT - III: Irreversible Thermodynamics (18 Hours)

Local equilibrium theory of thermodynamics – Principal aims of classical irreversible thermodynamics – Transport equations – Fourier's law, Fick's law and Ohm's law. Concept of nonequilibrium states and processes; Criterion of irreversibility with reference to entropy – Entropy flow and entropy production in irreversible processes – linear flux-force relations. Phenomenological laws and Linear laws– Onsager's reciprocity relations, applications to electrokinetic phenomena, Coupled phenomena - Peltier and Seeback effects, Curie's theorem – Prigogine's principles of minimum entropy production. Derivations and calculation of changes in entropy as phase changes. Concepts of absolute entropies – determination of heat capacity and molar entropy of molecular oxygen existing in different states.

UNIT - IV: Kinetics of Chemical Reactions (15 Hours)

Comparison of gas phase and solution reactions, kinetics of homogeneous reactions in solution –ion-ion, ion-dipole and dipole-dipole reactions; linear free energy relationships – Hammett, Taft and Marcus equations; solid state reactions; reactions of molecular beams; diffusion-controlled reactions. Unimolecular reactions – Lindemann theory; Chain reactions – rate laws – decomposition acetaldehyde, Thermal and photochemical reactions involving H_2+-Cl_2 and H_2-Br_2; The H_2-O_2 reaction – explosions; Homogeneous catalysis – Acid – base catalysis – Bronsted catalysis law. Theories of reaction rate – absolute reaction rate theory; Steric factor.

UNIT-V: Kinetics of Electrode Processes (15 Hours)

Mechanism of electrode reactions – multistep electron transfer reactions, significance of equilibrium exchange current density and transfer coefficient; mechanism of hydrogen evolution and oxygen evolution reactions. Corrosion of Metals – mixed potential mechanism – different types of corrosion – methods protection of metals from corrosion.

Reference Books:

1. M.C. Gupta, Statistical thermodynamics Wiley Easter, New Delhi, 1990.
2. K.J. Laidler, Chemical Kinetics,
3. J.O'M Bockris and A.K.N. Reddy Modern Electro Chemistry, Plenum
4. R.G. Pearson and J.W. Moore, Kinetics and Mechanism 3 edn, Wilely, 1981, 2.
5. C. Kalidas and M.V. Sangaranarayanan, Non- Equilibrium Thermodynamics.
6. Katchalsky, A. &Curren, P. F. Non-Equilibrium Thermodynamics in Biophysics, Harvard University, Press, Cambridge (1965).
7. P.W. Atkins, Advanced Physical Chemistry, Chapter 5, Entropy, Absolute entropies and 2nd& 3rd laws of Thermodynamics.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://www.youtube.com/watch?v=txOnRP5hwCE&list=PLwdnzlV3ogoX-

WIPb5DnmmmUOVAgI5wrq
2. https://www.youtube.com/watch?v=yBcz5Zaldus&list=PLdBDmcnzLC_ZMUWMdy7SmcTgnnzyiRpql
3. https://www.youtube.com/watch?v=sYY6HgNC8mY&list=PLyqSpQzTE6M9fKXkUtjhcyWNpeJUSbter
4. https://www.youtube.com/watch?v=zxgJst95eIg
5. https://www.youtube.com/watch?v=fZUU42KlwCA

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	M	M	L	M	S	M	L	S	M
CO 2	M	M	S	L	M	L	M	S	L	S
CO 3	S	S	M	M	S	S	M	L	M	M
CO 4	M	M	S	L	M	L	M	S	M	L
CO 5	M	S	M	S	M	S	M	L	M	S

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C307**	**Advanced Quantum Chemistry and Applied Materials**	**4**

Course Objectives:

The main objectives of this course are,

- To provide advanced knowledge and problem solving skill in theory and applications of quantum chemistry.
- To learn applications of solid state material in terms of band theory, electrical, magnetic and optical properties of solids.
- To give advanced knowledge on the synthesis, characterization and applications of polymers.
- To know the background and applications of different applied materials, and its current research scenario.
- To develop the ability to do some independent research problems and use some experimental resources at the end of the course.

Pre-requisites, if any:

Students should know the fundamental aspects of quantum chemistry, solid state chemistry, polymer chemistry along with problems solving.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall advances in quantum chemistry and fundamental aspects of polymer chemistry and material chemistry. (**K1**)
- **CO2:** Understand the recent progress of quantum chemistry, polymer chemistry and material chemistry. (**K2**)

- **CO3:** Apply the knowledge of quantum chemistry, polymer chemistry and material chemistry to different areas of chemistry. (**K3**)
- **CO4:** Analyze and Evaluate the research problems in quantum chemistry, polymer chemistry and material chemistry. (**K4** and **K5**).
- **CO5:** Create new concepts to expand the dimension quantum chemistry, polymer chemistry and material chemistry. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Theory and Principles **(14 Hours)**

Particle in a box, quantum mechanical tunneling, solution of Schrodinger equation forharmonic oscillator and rigid rotator, quantum mechanical treatment of hydrogen atom, radial and angular wave function, approximation methods – perturbation method and variation method, application to helium.

Electron spin-Spin angular momentum, spin orbital, eigen values of spin angular momentum, normalization and orthogonality relations, Many electron atoms – Hamiltonian and wave functions, Slater determinants, symmetry and antisymmetric wave functions, application of Pauli exclusion principle to He atom and excited He atom, Viral theorem and its applications to chemical bonding, Hellman-Feynmann theorem, electrostatic theorem.

UNIT - II: Applications in Bonding **(10 Hours)**

MO treatment of hydrogen molecule ion and hydrogen molecule, VB treatment of hydrogen molecule. MO treatment of simple mono nuclear and hetero nuclear diatomic molecules, HMO treatment of ethylene butadiene and benzene, Hartree Fock SCF MO treatment, semi empirical SCF MO theory, Walsh diagrams.

UNIT - III: Solid State and Advanced Catalysis **(15 Hour)**

Quantum Mechanical description of solids, Free electron approximation, band model, Fermi Dirac distribution, Band model applied to metals, semiconductors and insulators, Semiconductors – intrinsic and impurity semiconductors, Defects in Solids, Defect equilibria, Electrical, magnetic and optical properties of solids. Low-dimensional solids; superconductivity; Molecular electronics.

Catalysis Homogeneous catalysis, reactions, Turn over number, Turn over frequency, Heterogeneous catalysis, Zeolites, AlPOs, Mesoporous materials, Straight-run gasoline, cracked gasoline, Catalytic cracking of heavy oil, Catalytic reforming of naphtha, Hydrodesulphurization, Hydrodenitrogenation, Hydrodeoxygeantion, synthesis of fine chemicals.

UNIT - IV: Macromolecules **(10 Hours)**

Polymerization techniques – types of polymerization – condensation addition – ionic – coordination – stereospecific copolymerization – grafting.

Kinetics of polymerization (ionic and addition) – Kinetics of copolymerization – Mechanism of polymerization – chain initiation, propagation, termination, transfer – inhibition and retardation.

Properties of polymers – molecular weight of polymers, Mw &Mn Determination – osmometry, light scattering, viscosity, and ultracentrifuge – get permeation chromatography. Crystallinity of polymers – glass transition temperature – polymers as materials.

UNIT - V: Applied Materials **(11 Hours)**

Dye sensitized and perovskite solar cells, photocatalysis and electrocatalysis, OLED materials, Mesoporous materials, Metal-organic frameworks, Carbon capture and storage, Bioimaging, Drug delivery, Ionic liquids, Liquid crystals.

Reference Books

1. Quantum chemistry, Eyrimg, Walter and Kimball.
2. Mathematics for physics and chemistry margenau and Murphy.
3. K.J.Laidler, physical chemistry with biological applications, Benjamin/Cummings publishing Co, 1978.
4. R.Chang, physical chemistry with application to biological systems, MacMillan publishing Co, London, 1977.

Text Books

1. Molecular quantum mechanics, P.W. Atkins, Oxford University press 1983.
2. Quantum mechanics in chemistry, M.W. Haung, W.A. Benjaamen.
3. Introduction to solid state physics, Kittel.
4. Solid state chemistry, N.B. Hannay.
5. Introduction to solids, Azareff Prentice Hall- TMH.
6. Band theory of metals, S.L. Altmann, Pergamon, 1970.
7. F.W. Billmeyer, Text Book of polymer science Wiley Interscience, 1984.
8. A. Rudin, the elements of polymer science and engineering. An introductory text for engineers and chemists, Academic Press, New York, 1982.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://www.youtube.com/watch?v=G2zgAs5O7I8
2. https://www.youtube.com/watch?v=_eak-XY3Vx8
3. https://www.youtube.com/watch?v=7ct8QsBn5G8
4. https://www.youtube.com/watch?v=jSNlmOwpxYg&list=PLbMVogVj5nJT0slH3tuas5BIp1DG8ZpMj
5. https://www.youtube.com/watch?v=5zAQot4pKgU&list=PLLy_2iUCG87Dxsmc322YcSuNl_KCEbqPl
6. https://www.youtube.com/watch?v=YvcGL3J9_IM

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	S	M	L	M	S	M	L	M	S
CO 2	M	M	S	M	S	L	M	S	L	S
CO 3	S	M	M	S	M	S	M	L	M	L
CO 4	S	S	M	S	L	M	S	M	S	M
CO 5	M	M	S	M	S	L	M	S	L	S

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Elective	**CHE E004**	**Electroanalytical Chemistry**	**3**

Course Objectives:

The main objectives of this course are to,

- Learn the theory and basics of electrochemical techniques and their applications.
- Design and understand functioning of electrochemical sensors.
- Gain knowledge on Electrochemical Impedance Spectroscopy.
- Describe the theory and practical applications of voltametric techniques and polarography.
- Understand the principles and applications of coulometry and electrogravimetry.

Pre-requisites, if any:

Students should know the fundamental aspects of electrochemistry along with problems solving skill.

Course Outcomes:

On the successful completion of the course, student will be able to have,

- **CO1:** Working knowledge on sensors and electrochemical impedance spectroscopy. (**K1-K4**)
- **CO2:** Better understanding of Types of electrodes and their functions. (**K3-K5**)
- **CO3:** Knowledge on electrical double layer and electrokinetic properties. (**K2-K4**)
- **CO4: T**he principles and applications of different types of voltammetric and polarographic techniques. (**K2-K5**)
- **CO5: S**kill and confidence to apply electroanalytical techniques to research. (**K3-K4**)
- **CO6:** The fundamentals of corrosion and its prevention. (**K5 & K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Electrical Double Layer, Corrosion and Electrokinetic applications (15 Hours)

Electrical double layer – Electrode - electrolyte interface, Types of interfaces, thermodynamics of electrified interfaces, derivation of electrocapillary phenomena, Point of Zero Charge (PZC), Lippmann equation, estimation of surface charge and surface excess and Gibbs adsorption. Structure of electrified interfaces, Helmholtz-Perrin, Gouy – Chapman and Stern models, specific adsorption. Corrosion - Thermodynamic criteria of corrosion of metals – Dry and wet corrosion, homogenous (Wagner and Traud's) and heterogenous theories, classification of corrosion –Uniform, Galvanic, Crevice, Pitting and Intergranular corrosion- Povrbaix diagram. Corrosion prevention - passivation and inhibitors. Electrokinetic phenomena - overview of Zeta Potential – Principles, Mechanism and applications. Conversion and storage of electrochemical energy. Fuel cells and Lithium-ion battery.

UNIT - II: Potentiometric and sensing techniques (15 Hours)

Potentiometry - standard and formal potentials - Nernst equation. Types of electrodes - indicator and reference electrodes. Ion selective electrodes - crystalline and non crystalline electrodes - glass electrode for pH measurements, mechanism of electrode response and evaluation of selectivity coefficient, asymmetry potential, alkaline and acid errors, applications of ion selective electrodes. Chronoamperometry and Chronopotentiometry. Potentiometric titrations - manual and automatic titrators, titrations including differential methods titrations in non-aqueous systems, titrations with polarized electrodes. Bipoteniometry - principle, instrumentation and applications. Amperometric and Potentiometric sensors - Gas Sensors, Bio sensors.

Impedance spectroscopy, RDE, RRDE, sensors

UNIT - III: Voltametric Techniques (15 Hours)

Voltammetry–Polarography- DME, polarograms, currents in polarography, polarographic maxima, effect of dissolved oxygen and application to chemical analysis, amperometeric titrations, pulse polarography – normal and differential pulse, square wave polarography, stripping methods – cathodic and anodic stripping, linear sweep voltammetry, cyclic voltammetry, types of electrodes and chemically modified electrodes. Coulometric analysis - Theory, Faraday's laws, types of coulometres, coulometric titrations; Electrogravimetry – Theory, electrogravimetry, order of deposition, constant potential, constant current deposition and deposition of complex ions.

Contemporary Issues:

Expert lectures, YouTubes Videos, Animations, NPTEL, MOOC videos, online seminars – webinars for strengthening the subject matters.

Text Books:

1. Douglas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition.
2. A. M. Bond, Modern polarographic methods in Analytical Chemistry, Marcel Decker Inc., 1980.
3. Principles of Instrumental Analysis – Douglas A. Skoog, F. Holler, Stanley Crouch, 7th Edn Brooks/Cole publish; 7th edition, 2017.
4. E. Gileadi, E. Kirowa- Eisner and J. Penciner, 3. Interfacial Electrochemistry: An Experimental Approach, Addison-Wesley Publishing Company, Massachusetts,1975.
5. P.T. Kissinger and W.R. Heineman, 8. Laboratory Techniques in Electroanalytical chemistry, Marcel Decker Inc., 1984.

Reference Books:

1. John O'M. Bockris, Amulya K. N. Reddy, "Modern Electrochemistry", Vol. I and II, Plenum Publishing, 2008.
2. John O' M.Bockris&A.K.N.Reddy, Modern Electrochemistry – Fundamentals of Electrodics, Plenum Publishers, New York, 2000.
3. Willard, H.H.; Merritt, L.L. Jr.; Dean, J.A.; Settle, F.A. Jr., CBS Publishers & Distributors; 7th edition (2004).
4. Modern polarographic methods in Analytical Chemistry- A. M Bond, Marcel Decker Inc.,

1980.
5. Laboratory Techniques in Electroanalytical chemistry – P.T. Kissinger and W.R. Heineman, Marcel Decker Inc., 1984.
6. Chemical Instrumentation – H.A. Stoubel, Addison- Wesley, 1976 Stripping analysis – J. Wang, VCH Publication, 1985.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites, etc.]:

1. https://www.youtube.com/watch?v=3olOk_xNq8g
2. https://www.youtube.com/watch?v=l2ENx_Y0dNU
3. https://www.youtube.com/watch?v=_bRI2bv_YqY&list=PLyqSpQzTE6M9ftJKyUWBilfrgBjh_6eh1

Course Designed By:
Dr. Deepa P Nambiar, Dr. P. Prabhu and Dr. A. Murugadoss

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	M	S	S	M	M	S	M	M	L	L
CO 2	S	M	S	S	M	M	S	M	L	L
CO 3	S	M	S	M	L	M	S	L	L	L
CO 4	M	S	S	S	L	S	M	L	L	L
CO 5	S	S	S	M	L	L	S	L	L	L
CO 6	S	M	S	S	M	M	S	M	L	L

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Core	**CHE C308**	**Project**	**6**

Course Objectives:

The main objectives of this course are,

- To understand and identify new research problems in chemistry.
- To collect literature in the identified research area using scientific resources.
- To design the new synthetic scheme or protocol based on the literature search.
- To execute experiments to collect and analyze the data.
- To prepare the research report based on the obtained results.

Pre-requisites, if any:

Students should select are of research and have to give a research proposal on this to respective guide.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall the basics of chemistry for choosing a research problem. (**K1**)

- **CO2:** Understand the methodologies for collecting literature search. (**K2**)
- **CO3:** Apply the knowledge for systematic execution of the research work. (**K3**)
- **CO4:** Analyze and Evaluate the research data with reference to literature. (**K4** and **K5**)
- **CO5:** Create new research report based on the outcome of research work. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

Detailed Syllabus **(270 Hours)**

Departmental Committee will allot a stipulated number of projects to Individual faculty members. Guide allotment for the M.Sc. project will be based on lot basis. The allotted students have to consult respective faculty members and select project topic.

Once guide allotment is declared, the student has to submit a research proposal followed by presentation to the respective guide. Students will be periodically assessed for their project work by the individual faculty member.

The final submission of the research project i.e. small thesis, presentation, and comprehensive viva carries 100% marks.

Note:

1. Student should submit 3 copies of the final research project copy in hard binding format with all declarations and signatures.
2. For referencing any ACS journal pattern should be followed.

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	M	M	S	M	M	S	M	M	S	S
CO 2	S	S	M	L	S	M	L	M	L	M
CO 3	S	M	S	M	S	L	S	S	L	S
CO 4	M	S	M	L	M	M	M	M	S	L
CO 5	S	M	M	S	M	S	L	S	L	M

Core/ Elective/ Supportive	Course Code	Title of the Course	Credits
Elective	**CHE E303**	**Macromolecular Chemistry - II**	**3**

Course Objectives:

The main objectives of this course are,

- To provide analytical skill to analysis and testing of polymer by FT-IR, NMR, XRD, TGA/DTA/DSC.
- To give knowledge on synthesis and reactions of vinyl polymers.
- To know synthesis of polyethers, polysulfides and its related polymers.
- To understand the synthesis of polyesters, polyamides and related polymers.
- To recognize the synthesis of heterocyclic, inorganic and miscellaneous organic polymers.

Pre-requisites, if any:

Students should know the UG level fundamental aspects on polymer chemistry.

Course Outcomes:

After completion of this course successfully, the students will be able to,

- **CO1:** Recall the techniques of polymer characterization. (**K1**)
- **CO2:** Understand the synthesis of vinyl and nonvinyl polymers. (**K2**)
- **CO3:** Apply the synthetic knowledge of polymers in diverse areas of basic sciences. (**K3**)
- **CO4:** Analyze and Evaluate the synthetic methodologies to obtain desired polymer products. (**K4** and **K5**).
- **CO5:** Create synthetic strategies for developing new polymeric materials. (**K6**)

K1 - Remember; **K2** - Understand; **K3** - Apply; **K4** - Analyze; **K5** - Evaluate; **K6** – Create

UNITS

UNIT - I: Evaluation, Characterization and Analysis of Polymers (10 Hours)

Chemical methods of analysis, Spectroscopic methods of analysis – FTIR, Raman, NMR, EPR, UV-Visible and Fluorescence. Scattering methods of analysis - X-ray, electron and neutron. Characterization and analysis of polymer surfaces – SEM, AFM, ATR, photoacoustic spectroscopy (PAS), Electron spectroscopy for chemical analysis (ESCA) and secondary-ion mass spectrometry (SIMS) and Ion-scattering spectroscopy (ISS).

Thermal analysis – DSC, DTA, TGA, Thermomechanical analysis (TMA), Pyrolysis-gas Chromatography (PGC), Flammability testing.

Measurement of mechanical properties, Evaluation of Chemical resistance and electrical properties.

UNIT - II: Synthesis and Reactions of Vinyl Polymers (9 Hours)

Synthesis of vinyl polymers – Free radical polymerization and Ionic polymeriation, Vinyl polymerization with complex coordination catalysts – Homogeneous and Heterogeneous Ziegler-Natta polymerization, Reactions of vinyl polymers – Functional group reactions, Ring-forming reactions, Crosslinking, Block and graft copolymer formation and polymer degradation.

UNIT - III: Synthesis of Nonvinyl Polymers - I (8 Hours)

Step-reaction and ring-opening polymerization, Preparation of polyethers by chain-reaction and ring opening polymerization, Preparation of polyethers by chain-reaction, ring opening and step-reaction polymerization, Synthesis of polysulfides, poly(alkene polysulfide)s and polysulfones.

UNIT - IV: Synthesis of Nonvinyl Polymers - II (9 Hours)

Synthesis of polyesters – linear, hyperbranched and crosslinked polyesters. Synthesis of polyamides and related polymers – Polyamides, polyureas, polyurethanes, polyhydrazides, polyimides.

UNIT - V: Synthesis of Nonvinyl Polymers - III (9 Hours)

Synthesis of phenol-, urea- and melamine-formaldehyde polymers, Synthesis of heterocyclic and inorganic polymers.

Synthesis of miscellaneous organic polymers – polycarbodiimides, polyamines, polymers containing carbon-carbon double and triple bonds, azo polymers, poly(p-phenylene), poly(p-

xylylene), polyanhydrides, polyamines, Friedel-Crafts polymers, Charge transfer polymers and ionic polymers.

Text Books:

1. Malcolm P. Stevens, Polymer Chemistry Introduction, 3rd edition, 2011.
2. F.W. Billmeyer, Text Book of polymer science Wiley Interscience, 1984.
3. A. Rudin, the elements of polymer science and engineering. An introductory text for engineers and chemists, Academic Press, New York, 1982.
4. M.S. Bhatnagar, A Textbook of Polymers. Vol I. S.Chand & Company Ltd 2004.
5. A. Bill Meyer, Text Book of Polymer Chemistry, Singapore: John Wiley & Sons 1994,
6. E.C. Carraher, Introduction to Polymer Chemistry. Taylor & Francis, Inc. 2006.
7. Gowariker & Viswanathan, Polymer Science. Wiley Eastern, 1986.
8. S.P. Mishra, Polymer Chemistry. New Delhi: Wiley Eastern Ltd 1993.

Related Online Contents [MOOC, SWAYAM, NPTEL, Websites etc.]

1. https://www.youtube.com/watch?v=sQypNsEwsM8&list=PLcCIZORoVQghF126hJD0yU6JZ6ngbOb5a
2. https://www.youtube.com/watch?v=r1f4_0XSN0k
3. https://www.youtube.com/watch?v=8jaxr0RhYPU
4. https://www.youtube.com/watch?v=VGRpdv6S-0I

Mapping with Programme Outcomes: (S-Strong, M-Medium, L-Low)

	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PO 8	PO 9	PO 10
CO 1	S	S	M	M	S	M	M	S	M	S
CO 2	S	M	S	M	M	M	S	M	M	S
CO 3	M	S	L	S	M	S	M	L	S	M
CO 4	M	S	L	L	M	M	S	M	S	M
CO 5	M	M	S	S	S	M	S	M	M	S