MANONMANIAM SUNDARANAR UNIVERSITY TIRUNELVELI – 12

Vision

"To provide quality education to reach the un-reached"

Mission

- To conduct research, teaching and outreach programmes to improve conditions of human living
- To create an academic environment that honours women and men of all races, caste, creed, cultures and an atmosphere that values intellectual curiosity, pursuit of knowledge, academic freedom and integrity
- To offer a wide variety of off-campus educational and training programs, including the use of information technology, to individuals and groups.
- To develop partnership with industries and government so as to improve the quality of the workplace and to serve as catalyst for economic and cultural development
- To provide quality / inclusive education, especially for the rural and un-reached segments of economically downtrodden students including women, socially oppressed and differently abled

SRI PARAMAKALYANI CENTRE OF EXCELLENCE IN ENVIRONMENTAL SCIENCES

Vision

The Sri Paramakalyani Centre of Excellence in Environmental Sciences was established in Alwarkurichi in 1992. The genesis of the centre can be traced to the historical judgment of the Hon'ble Supreme Court in the case of M.C.Mehta VS Union of India and others, where the introduction of Environmental Education at undergraduate and postgraduate levels was made mandatory.

The centre faithfully adheres to the vision enshrined in the constitution of India that is" to protect and improve the natural environment including forests, lakes, rivers, and wildlife" and to "develop the scientific temper humanism and spirit of inquiry and reform. To make these lofty ideals the centre envisages developing in-depth knowledge of and technologies suitable for the country.

MANONMANIAM SUNDARANAR UNIVERSITY TIRUNELVELI – 12

Sri Paramakalyani Centre of Excellence in Environmental Sciences

M.Sc. NANOSCIENCE (CBCS)

REVISED AND RESTRUCTURED SYLLABI

(Effective from the academic year 2022-2023 onwards)

1. Course: **Nanoscience (MSc.)**
2. Duration: **Two Years Full Time (Each Year having Two Semesters)**
3. Medium of Instruction and Examinations: **English**

4. Eligibility for Admission:

A candidate shall be eligible for admission to Nanoscience (M.Sc) course if he/she has obtained Bachelor's degree (B.Sc., Nanoscience, Nanochemistry, Physics, Chemistry, Applied Chemistry, Organic Chemistry, Inorganic chemistry, Physical Chemistry, Analytical Chemistry, Industrial Chemistry, Textile Chemistry, Nanobiology, Nanophysics, Nanobiochemistry, Nanoscience and Nanotechnology, Life Sciences in equivalent degree recognized by our university with a minimum of fifty percent (50%) marks (For SC/ST – Pass).

5. **Scheme of the course – (For I – IV Semesters)**

Course Structure

Semester	Subject No	Subject Status	Subject	Hours/ Week	Credits	Marks		
						Int	Ext	Total
I	1	Core – 1	Introduction to Nanoscience	4	4	25	75	100
	2	Core – 2	Reaction mechanism and Stereochemistry	4	4	25	75	100
	3	Core – 3	Chemical kinetics and electrochemistry	4	4	25	75	100
	4	Practical –1	Introduction to Nanoscience – Practical	3	2	50	50	100
	5	Practical – 2	Reaction mechanism and stereochemistry and chemical kinetics and electrochemistry – Practical	3	2	50	50	100
	6	Skill Based Core (Mandatory)	E-Pathshala (Analytical Chemistry)	2	2	25	75	100
	7	Elective-1	Any One 1. Advances in Nanobiotechnology 2. Scientific Research Methodology 3. Green Chemistry	3	3	25	75	100
	Subtotal			**23**	**21**	**225**	**475**	**700**

Semester	Subject No	Subject Status	Subject	Hours/ Week	Credits	Marks		
						Int	Ext	Total
II	8	Core – 4	Synthesis of Nanomaterials	4	4	25	75	100
	9	Core – 5	Structure and bonding	4	4	25	75	100
	10	Core – 6	Quantum chemistry and analytical techniques	4	4	25	75	100
	11	Practical –3	Synthesis of Nanomaterials – Practical	3	2	50	50	100
	12	Practical – 4	Structure and bonding and quantum chemistry and analytical techniques – Practical	3	2	50	50	100
	13	Supportive Course (Mandatory)	Online Course from Swayam, MOOCs, NPTEL etc.	3	3	25	75	100
	14	Elective-2	Any One 1. Industrial Nanotechnology 2. Applied Chemistry 3. IPR and Biosafety	3	3	25	75	100
	15		Field Work		2	50	50	100
	Subtotal			**24**	**24**	**275**	**525**	**800**

Semester	Subject No	Subject Status	Subject	Hours/ Week	Credits	Marks		
						Int	Ext	Total
III	16	Core – 7	Reaction mechanism, rearrangement, name reactions, oxidation and reduction	4	4	25	75	100
	17	Core – 8	Coordination chemistry	4	4	25	75	100
	18	Core – 9	Thermodynamics and group theory	4	4	25	75	100
	19	Practical –5	Reaction mechanism, rearrangement, name reactions, oxidation and reduction – Practical	3	2	50	50	100
	20	Practical – 6	Coordination chemistry and thermodynamics and group theory – Practical	3	2	50	50	100
	21	Elective-3	Any One 1. Introduction to Nanotoxicology 2. Computational Nanoscience 3. Nanocomposite	3	3	25	75	100
	22	MOOCs	Online Course from Swayam, MOOCs, NPTEL etc.	3	3	25	75	100
	23		Mini Project		3	50	50	100
	Subtotal			**24**	**25**	**275**	**525**	**800**

Semester	Subject No	Subject Status	Subject	Hours/ Week	Credits	Marks		
						Int	Ext	Total
IV	24	Core – 10	Photochemistry, pericyclic reactions, heterocycles and natural products	4	4	25	75	100
	25	Core – 11	Inorganic photochemistry, spectroscopy and organometallics	4	4	25	75	100
	26	Core – 12 (E-Pathshala)	Environmental Chemistry	3	3	25	75	100
	27	Core-13	Applications of Nanotechnology	4	4	25	75	100
	28	Internship	Industrial Internship		4	50	50	100
	29	Project	Project & Viva – Voce	4	6	50	50	100
	Subtotal			**19**	**25**	**200**	**475**	**600**
	Grant Total			**90**	**95**	**975**	**2000**	**2900**

DISTRIBUTION OF CREDIT:

CORE	12 X 4	**48**
PRACTICALS (Core)	6 X 2	**12**
ELECTIVE	3 X 3	**9**
SUPPORTIVE COURSE (Mandatory)	1 X 3	**3**
SKILL BASED COURSE (Mandatory)	1 X 2	**2**
FIELD WORK	1 X 2	**2**
MOOCs	1 X 3	**3**
MINI PROJECT	1 X 3	**3**
INDUSTRIAL INTERNSHIP	1 X 4	**4**
PROJECT AND VIVA-VOCE	1 X 6	**6**
TOTAL NO OF CREDITS		**92**
TOTAL NO MARKS		**2800**

1. For each theory paper 25 marks for internal & 75 marks for External.
2. There is no passing minimum for internal examination. Passing minimum for external is 50% and the total passing minimum including external & internal is altogether 50%. For internal marks, the split up is 15 marks for test, 5 marks for seminar and 5 marks for Assignment. The average of all three tests will be taken for test marks.
3. For project valuation 25 marks maximum for internal and 75 marks maximum for external and Viva Voce and thereby the total maximum for project valuation is 100. **Grant Total for Project + Viva Voce is (25+75) 100 marks.**
4. The question paper pattern for theory exam is as follows:

SECTION A – 10 x 1 mark –10 marks

(Two questions from each unit)

SECTION B – 5 X 5marks – 25 marks

(One question from each unit with either or choice)

SECTION C – 5 X 8 marks – 40 marks

(One question from each unit with either or choice)

Total 100 marks

PRACTICAL EXAMINATIONS - QUESTION PAPER PATTERN:

QUESTIONS	INTERNAL – 50 marks	EXTERNAL–50 marks	TOTAL
1. MAJOR	15	15	30
2. MINOR	10	10	20
3. SPOTTERS	15 (5 spotters, each 3 marks)	15 (5 spotters, each 3 marks)	30
4. RECORD	5	5	10
5. Viva-voce	5	5	10
TOTAL	**50**	**50**	**100**

Programme Outcomes (POs)

On successful completion of M.Sc. Nanoscience programme, the student will be able to

PO-1: Demonstrate comprehensive knowledge and skills in different areas of Chemistry, viz; Organic, Inorganic, Physical, Analytical and Materials Chemistry

PO-2: Apply knowledge and experimental skills to synthesize and analyze chemicals/Materials of immediate need for the society and analyze chemical problems.

PO-3: Critically evaluate practices, rules, and theories based on empirical evidence, by following the scientific approach to knowledge development in Chemistry.

PO-4: Demonstrate effective communication skills both orally and in writing using appropriate media in all the aspects related to Chemistry and one's profession

PO-5: Demonstrate a sense of inquiry and ability to define problems; design methodology, analyze, evaluate and resent report on innovative scientific research problems.

PO-6: Apply the knowledge of chemistry associated with critical thinking to achieve sustainable solutions for energy and environment and other problems in day-today life.

PO-7: 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-8: Demonstrate knowledge of the values of multiple cultures and a global perspective effectively engage in a multicultural society for employment or further studies. Pursue higher education / employable / entrepreneur.

Programme Specific Outcomes (PSOs)

Upon successful completion of M.Sc. Chemistry programme, the student will be able to

PSO1: Gain comprehensive knowledge and understanding of fundamental concepts, applications of chemical and various scientific theories; skills in Organic, Inorganic, Physical, analytical nano

science, environmental, biological chemistry and Materials Chemistry and other modern areas of Chemistry.

PSO2: Understand the background of organic /inorganic reaction mechanisms, chemical structures and experimental methods of chemical analysis, organic synthesis, molecular rearrangements and separation techniques.

PSO3: Use ideas, and techniques of chemistry and other fields of science to acquire knowledge in the emerging areas of science.

PSO4: Gather deep understanding about the physical aspects of atomic structure, quantum theory, molecular spectroscopy, thermodynamics, kinetics, catalysis, chemical equilibrium, reaction pathways with respect to time, various energy transformations, molecular assembly at surface level, significance of electrochemistry, and molecular segregation using their symmetry.

PSO5: Appreciate the importance of various elements in the periodic table, coordination chemistry and structure of molecules, properties of compounds, structural determination of molecules /complexes using theories and experimental techniques.

PSO6: Use technologies/instrumentation to acquire and analyze data of chemical systems in a sophisticated laboratory environment to secure challenging positions in industry, academics and government sectors by learning various analytical techniques such as UV, IR, NMR, MS, Chromatography etc and their applications.

PSO7: Develop skills in literature survey, designing synthetic methodologies and characterizing the ventured compounds; Prepare for self-learning and lifelong-learning to meet one's learning needs using research and development work and professional materials.

PSO8: Transform learned knowledge and skills to qualify in the NET and other national and international level competitive exam for higher studies and jobs

FIRST SEMESTER

Core – 1: INTRODUCTION TO NANOSCIENCE

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. To study the relationship between the size and properties of nanomaterials
2. To understand the growth mechanisms of nanocrystals
3. To understand the different types of Nano systems and nanomaterials

Course Prerequisites:

Obtain basic knowledge in nanoscience.

Course Outcomes (Cos):

At the end of the course, the student will be able to

CO1: Remember key concepts of nanoscience and nanotechnology. The Basic concept, methods and techniques of nanoscaffolds

CO2: Understand how nanotechnology can be tailored and used for biomedical purposes, catalyst.

CO3: explain the properties of nanomaterials are size dependent. Predict the behavior of nanomaterials

CO4: demonstrate the approaches to design and fabrication of nanomaterials

CO5: summarise the scientific method and justify its use in science

Course Outline:

UNIT I **9Hrs**

Scientific revolution- Atomic Structures-Molecular and atomic Size-Bohr radius – Emergence of Nanotechnology – Challenges in Nanotechnology – application area. Scope of nanoscience and technology. Carbon age–New form of carbon (from Graphene sheet to CNT).

UNIT II **9Hrs**

Surface to volume ratio. Surface properties of nanoparticles. Mechanical, optical, electronic, magnetic, thermal and chemical properties of nanomaterials. Size dependent properties-size dependent absorption spectra.

Top-down and bottom-up approaches-self-assembly process-grain boundary volume in nanocrystals-defects in nanocrystals-surface effects on the properties, Influence of nucleation rate on the size of the crystals

UNIT III **9Hrs**

Definition of a Nano system - Types of Nanocrystals-One Dimensional (1D)-Two Dimensional (2D) -Three Dimensional (3D) nanostructured materials - Quantum dots – Quantum confinement – thin films- Quantum Wire-Core/Shell structures.

UNIT IV **9Hrs**

Quantum dots-optical properties and applications. Carbon Nano tubes-type, physical properties and applications. Magnetic behaviour of nanomaterials. Electronic transport in quantum wires. Surface chemistry of tailored monolayer.

UNIT V **9Hrs**

Properties of Individual Nanoparticle - Metal Nanoclusters- Semiconducting Nanoparticle- Rare Gas and molecular Clusters- Method of synthesis - RF plasma- Chemical methods- Thermolysis - Pulsed Laser Methods.

Mapping of Cos to POs and PSOs

CO		Correlation level																Cognitive level
		PO								PSO								
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K1
CO2	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K2
CO3	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K3
CO4	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K4
CO5	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K5

References

1. W. Rainer, Nano Electronics and information Technology, Wiley, 2003.
2. K.E.Drexler, Nano systems, Wiley, 1992.
3. G.Cao, Naostructures and Nanomaterials: Synthesis, properties and applications, Imperical College Press, 2004
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5. M. Wilson, K. Kananga, G Smith, M. Simmons, B. Ragusa, Nanotechnology: Basic science and Emerging technologies, Overseas Press India Pvt Ltd, New Delhi, First Edition, 2005
6. C.N.R. Rao, A.Muller, A.K.Cheetham (Eds), The chemistry of nanomaterials: Synthesis, properties and applications, Wiley VCH Verlag Gmbh&Co, Weinheim, 2004.

7. C.S.S.R.Kumar, J.Hormes, C.Leuschner, Nanofabrication towards biomedical applications, Wiley –VCH Verlag GmbH & Co, Weinheim, 2004.

8. Mick Wilson, Kamali Kannargare., Geoff Smith, "Nano technology: Basic Science and Emerging technologies", Overseas Press, 2005.

9. Charles P. Poole, Frank J. Owens, "Introduction to Nanotechnology", Wiley Interscience, 2003.

10. Mark A. Ratner, Daniel Ratner, "Nanotechnology: A gentle introduction to the next Big Idea", Prentice Hall P7R:1st Edition, 2002.

11. T. Pradeep, "Nano the Essential Nanoscience and Nanotechnology", Tata McGraw hill, 2007.

12. J. Dutta, H. Hoffmann, "Nanomaterials", Topnano-21, 2003.

Practical -1: INTRODUCTION TO NANOSCIENCE

L	T	P	C
-	-	3	2

1. Preparation of Self-Assembled Monolayers (SAM)
2. Spin coating method
3. Sol-gel method
4. Grain size determination
5. Determination of Molecular weight by viscometry method
6. To determine the Band-Gap of given Semiconductor using Four Probe Method.
7. Resistivity measurement of a thin film
8. Cyclic voltametric studies of the electrodes in different electrolytes
9. Image processing of SEM micrograph
10. Aqueous to organic phase transfer of Ag and CdS nanoparticles; confirmation by UV-Visible absorption

Core – 2: REACTION MECHANISM AND STEREOCHEMISTRY

Course Code:

L	T	P	C
4	-	-	4

Course Objectives:

1. Understanding the fundamental mechanism involved in electrophilic reactions, nucleophilic reactions and reactions that involve transient species.

2. Understanding the basic aspects of stereochemistry such as chirality, nomenclature, stereoselectivity Vs stereospecificity and Asymmetric synthesis.
3. Understanding the conformational analysis of six member ring systems.

Course Prerequisites:

Obtain basic knowledge in chemistry specialized in organic chemistry

Course Outcomes (Cos):

CO1: understanding kinetic and nonkinetic methods of determining organic reaction and their possible mechanisms.

CO2: Understand the possible mechanisms in aliphatic substitution reactions and the possible products. Also, they should be competent to think of competitive reactions that may lead to more than one product in such reactions depending upon various factors.

CO3: understand various types of reaction mechanisms involved in synthetic organic transformation.

CO4: Expected to write the resonance and other electronic factors and explain the ortho/para or meta directing effects of substituents in aromatic substation reactions. Also ,the students are expected to identify and explain such reactions taking place in multistep organic synthesis

CO5: Understand the factors that are bringing about the difference in the mechanism of elimination reactions. They should be able to work out the product selectivity in varying types of elimination reactions with good understanding. Also the importance and appropriateness of carbonyl compounds in organic syntheses are to be explored by the students.

CO6: The students are expected to name the stereoisomers and draw their Sawhorse, Fisher and Newman Projection formulae. Gained knowledge of the relative stability and reactivity of conformational isomers in organic reactions.

Course Outline:

UNIT-I: Reaction mechanism **9Hrs**

Kinetic and Non kinetic methods of determining organic reaction mechanisms. Isolation and trapping of intermediates, Isotopic labeling studies. Primary Kinetic Isotopic effect. Generation of Kinetic and Thermodynamic enolates. Hammett equation-simple problems and Taft equation. Siginificance of reaction as well as substituent constants. Ambident nucleophiles such as CN-, NO_2-, phenoxide and ambident dianions. Williamsons ether synthesis.

UNIT-II: Aliphatic nucleophilic substitution **9Hrs**

Mechanism of nucleophlic substitution reaction: SN^1, SN^2 and SN^i mechanisms. Solvent and leaving group effects and neighbouring group participation (NGP). Substitution at carbonyl, vinylic and

bridgehead system. Substitution with ambient nucleophiles- "O" Vs "C"alkylation. Role of LDA, crown ethers and phase transfer catalysts (PTC) in nucleophilic substitution reactions.

Generation of enolates, enolate selectivity (Kinetic Vs Thermodynamic), alkylation of enolates and stereochemistry of enolate alkylation. Mechanism of ester hydrolysis (only BAc^2, AAc^2 and AA^{l1}). Alkylation of active methylene compounds. Asymmetric alkylation (Evans, Enders and Meyers procedures). Preparation and synthetic utility of enamines, Finkelstein reaction, Wurtz coupling.

UNIT-III: Aromatic electrophilic and nucleophilic substitutions 9Hrs

Aromatic electrophilic substitution: mechanism of nitration, sulfonation, Friedel-Crafts alkylation and acylation reactions. Synthesis of di- and tri-substituted benzenes from benzene or mono-substituted benzenes. Hammett and Hammett-Taft equation. Haworth reaction (for naphthalene), Scholl reaction, Vilsmeier-Haack formylation, Gattermann reaction, Reimer-Tiemann and Bischler-Napieralski reactions.

Aromatic nucleophilic substitution in aryl halides by Meisenheimer complex mechanism and benzyne mechanism. Reactions of aryldiazonium salts. Zeigler alkylation, Vicarious Nucleophlic Substitution (VNS), Chichibabin and Schiemann reactions.

UNIT-IV: Reactive intermediates 9Hrs

Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, carbenoids, benzynes and nitrenes.

UNIT-V: Stereochemistry 9Hrs

Chirality, Symmetry elements, Asymmetric and Dissymmetric chiral molecules. Calculation of number of optical isomers. Stereochemistry of mono and di-substituted cyclopropane, cyclobutane, cyclopentane and cyclohexane. Stereochemistry of tri-substituted cyclopentane, tri-substituted pentane and tetra-substituted hexane. Description of various types of optically active compounds including allenes, cumulenes, spiranes, biphenyls, trans-cyclooctene.

Compounds containing two asymmetric centers; Erythro and threo isomers. Conversion of Fischer projection into perspective forms. Erythro and Threo-Inter conversion of Fischer to Sawhorse and Newman projections. Zig-Zag representation of glucose. Interpretation of homotopic, enantiotopic and diastereotopic atoms and faces. Pro-chiral carbon. Concept of Re- and Si- faces. R & S nomenclature of simple compounds, allenes, spiranes and biphenyls. Stereospecific and Stereoselective reactions. Asymmetric Synthesis-Crams rule and Felkin-Anh model. Conformational analyses of cyclohexane. di-substituted cyclohexanes and decalin.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1,K2
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5
CO6	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K6

References

1. Stereochemistry of Carbon compounds. (McGraw-Hill) E.L.Eliel
2. Organic Stereochemistry (McGraw-Hill) by Hallas.
3. Organic reaction mechanism (McGraw-Hill) R. K. Bansal.
4. Organic chemistry- R. T. Morrison and R. N. Boyd, (Prentice Hall.)
5. Modern organic reactions (Benjumin) H. O. House.
6. Principle of organic synthesis- R.O.C. Norman and J. M. Coxon.(ELBS)
7. Reaction mechanism in organic chemistry- S. M. Mukharji and S. P. Singh.
8. Stereochemistry of organic compounds c) D. Nasipuri.
9. Introduction to stereochemistry (Benjumin) K. Mislow.
10. Stereochemistry by P. S. Kalsi (New Age International)
11. Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 5th Ed, 2001.
12. F. Carey and R. J. Sundberg, Advanced Organic Chemistry-Part A and B, Springer Science + Business Media, 5 th Ed, 2007.
13. M. B. Smith and Jerry March, Advanced Organic Chemistry, John Wiley & Sons, 5th Ed, 2001.
14. J. Clayden, N. Greeves and S. Warren, Organic Chemistry, Oxford University Press, 2nd Ed, 2012.
15. M. B. Smith, Organic Synthesis, Academic Press, 3rd Ed, 2011.
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17. Stuart Warren, Organic Synthesis: Disconnection Approach, Wiley India (P) Ltd, 2007.
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19. E. N. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill Ed, Reprint 2008.
20. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International (P) Ltd, Reprint, 2005.

Core – 3: CHEMICAL KINETICS AND ELECTROCHEMISTRY

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. To understand the kinetics of chemical kinetics and explore the reaction kinetics of fast reactions
2. To learn the various techniques and mechanism of involved in catalysis.
3. To gain on understanding of the Ionic activity, ionic interactions, Debye-Hückel-Bjerrum model, Debye-Hückel limiting law.
4. To study the Debye-Hückel theory of strong electrolytes. To study the Electrical double layer, electrocapillary phenomena, surfactants.
5. The design and applications of the batteries and Fuel Cells, Corrosion and its Protection.

Course Prerequisites:

Basic knowledge in chemistry in the intermediate level with little knowledge in physical chemistry

Course Outcomes (COs):

CO-1: Understand the fundamental concepts on kinetics and reaction rate.

CO2: Develop knowledge on various theories of chemical kinetics.

CO3: Outline the effects of functional groups of biomolecules on metal-mediated biological reactions.

CO-4: Summarise the fundamental concepts and theories of electrochemistry and its application.

CO5: Apply the fundamental knowledge in kinetics, and electrochemistry to existing and emerging problem in basic science

CO-6: summarise the physical concepts of photochemistry

Course Outline:

UNIT-I: Chemical kinetics and catalysis **9Hrs**

Absolute reaction rate theory -Thermodynamic terms-Significance of entropy and volume of activation. Reactions in solution: factors determining reaction rates in solutions, effect of dielectric constant and ionic strength, - Bronsted –Bjerrum equation-Primary and Secondary salt effect, influence of solvent on reaction rates. Acid base catalysis-Bronsted relations, catalytic coefficients and their determination. Enzyme catalysis and its mechanism, Michaelis-Menten equation, effect of pH and temperature on enzyme catalysis, Mechanism of enzyme inhibition kinetics of surface reactions- unimolecular reactions-Bimolecular reactions-Langmuir Hinshelwood and Elay-Rideal mechanism.

UNIT-II: Chemical dynamics **9Hrs**

Potential energy surfaces-Dynamics of unimolecular reactions-Lindemann Hinshelwood, Rice-Ramsperger- Kassel (RRK) theory. Rice-Ramsperger-Kassel -Marsus (RRKM) theory.

Study of fast reactions by stopped flow techniques- relexation method, flash photolysis and the nuclear magnetic resonance method.

Linear free energy relationship-Hammett equation, Taft equation-Separation of polar, resonance and steric effects.

UNIT-III: Photochemistry **9Hrs**

Jablonski diagram, Primary and Secondary Processes, quantum yield and its determination-chemical actinometer. Excimers and exciplexes-Kinetics of collisional quenching-Stern Volmer equations. Photosensitization, Chemiluminescence. Photosynthesis, solar energy conversions. Semiconductor photo catalysis, lasers.

Radiation Chemistry-linear energy transfer, G-value, dosimeters, radiolysis of water, solvated electrons.

UNIT IV: Electrochemistry – I **9Hrs**

Deviation from ideal behaviour.ion-solvent and ion-ion interactions. Debye-Hückel-Bjerrum model, Ion association and triple ion formations. Expression for the mean activity coefficient.Debye-Hückel limiting law and its applications -Diverse ion effect. Van't Hoff factor and its relation to colligative properties. Debye-Hückel theory of strong electrolytes. Debye-Hückel length and potential around a central ion, its interpretation. Transport of ions in Solution: Electrolytic conduction- Debye - Hückel-Onsager treatment of strong electrolytes- ionic atmosphere- Anomalous conductance of non-aqueous electrolytes.

UNIT V: Electrochemistry- II **9Hrs**

Electrical double layer - Electrocapillary phenomena - Surfactants - Lipmann's equation, Electrokinetic phenomena.Zeta potential and its applications. Structure of electrical double layer – Helmholtz-Perrin, Guoy-Chapmann and Stern models. Butler-Volmer equation for one electron transfer reaction - equilibrium and exchange current densities- and symmetry factor - transfer coefficient.Cyclic voltammetry and Stripping voltammetry - principle – instrumentation- Corrosion and passivation of metals - Pourbaix diagram - Evans diagram –Batteries and Fuel cells-Ion selective electrodes.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1,K2
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5
CO6	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

References

1. Keith Oldham, Jan Myland and Alan Bond, Electrochemical Science and Technology: Fundamentals and Applications, John Wiley and Sons, New York, 2012.
2. G. L. Agarwal, Basic Chemical Kinetics, Tata McGraw Hill, 1990.
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4. Robert J Silbey, Robert A Alberty and Moungi G Bawendi, Physical Chemistry 4th Ed,NJ Hoboken: Wiley, 2015.
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6. Revise G. W. Castellan, Physical Chemistry, Narosa publishing House, New Delhi, Ed, 2011.
7. Gordon. M. Barrow, Physical Chemistry, Tata McGraw Hill Edition, New York, 2011.

8. L. R. Puri, Y. R. Sharma and R. S. Pathania, Principles of Physical Chemistry 46th Ed, 2012.

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Practical -2: REACTION MECHANISM AND STEREOCHEMISTRY AND CHEMICAL KINETICS AND ELECTROCHEMISTRY

L	T	P	C
-	-	3	2

Practical -2: Reaction Mechanism and Stereochemistry

A) Preparations

(One stage preparations involving various types of reactions)

1. Oxidation: Adipic acid by chromic acid oxidation of Cyclohexanol.
2. Aldol condensation: Dibenzal acetone from Benzaldehyde.
3. Sandmeyer reaction: p- Chlorotoulene from p-Toluidine.
4. Cannizzaro reaction: 4-chlorobenzyldehyde as a substrate.
5. Aromatic Electrophilic substitutions: Synthesis of p-Nitroaniline and p-Bromoaniline.
6. Synthesis of Heterocyclic compounds.
7. Synthesis of Dyes

B) Estimations:

1. Estimation of unsaturation.
2. Estimation of formalin.

3. Colorimetric Estimation of Dyes
4. Estimation of Amino acids (Any suitable Expt. may be added.)

Reference Books

1. A text book of practical organic chemistry- A. I. Vogel.
2. Practical organic chemistry- Mann and Saunders.
3. A handbook of quantitative and qualitative analysis- H. T. Clarke.
4. Organic Synthesis Collective Volumes by Blat.

Practical -2: CHEMICAL KINETICS AND ELECTROCHEMISTRY

Experiments are to be set up in the following techniques.

1. Potentiometry: Determination of solubility and solubility product of silver halides, determination of binary mixture of weak and strong acid etc.
2. Conductometry: Determination of mixture of acids and relative strength of weak acids.
3. Refractometry: Determination of molecular radius of molecule of organic compound.
4. Polarimetry: Kinetics of inversion of cane sugar in presence of strong acid.
5. Chemical Kinetics: Kinetics of reaction between bromate and iodide.
6. Partial Molar Volume: Determination of PMV by intercept method, density measurements etc.

Skill Based Core (Mandatory): ANALYTICAL CHEMISTRY (E-Pathshala)

L	T	P	C
2	-	-	2

Course Code:

Course Objectives:

Understand the Volumetric analysis compounds and their characters.

Study about Instrumentation methods.

Course Prerequisites:

The pre-requisite for studying the course on Analytical Chemistry is to have a basic skill in titrations, handling the apparatus and precaution in using the chemicals.

Course Outcomes (Cos):

CO-1: Be aware with calculations in analytical chemistry, be able to calculate titration errors for method evaluation, and perform statistical evaluation of results from classical and instrumental chemical experiments and analyses.

CO-2: Acquire the theoretical knowledge of the various spectroscopic methods on the basis of the examples from the science and industry, which are applied in industrial and scientific laboratories in the field of synthesis and structural determination

CO-3: Explain the theoretical principles of various separation techniques in chromatography, and typical applications of chromatographic techniques.

CO-4: Evaluate and suggest suitable electrochemical phenomena for a specific purpose, and evaluate sensitivity, important sources of interferences and identifications

CO5: summarise the significance of nanoscale & its dimensions, acquire knowledge of various characterization techniques, know the short term and longer term applications of material

CO6: develop the analytical skills of the students for handling instruments for quantitative analysis

Course Outline:

Unit 1 **9Hrs**

General analytical - Errors in analysis in laboratory safety- Volumetric analysis – Acid base titrations- Complexometric titrations- Redox titrations.

Unit 2 **9Hrs**

Precipitation argentometric titration - Gravimetric analysis - Mass spectrometry - Bomb calorimetry - Potentiometry - Ph. electrode, Membrane electrode, Biochemical electrode: ISFET, MOSFET.

Unit 3 **9Hrs**

Conductivity meter and salinity meter - DO meter – Polarography - Anode and cathode stripping voltammetry - Cyclic voltammetry - General chromatography, distribution coefficient and its implications.

Unit 4 **9Hrs**

Chromatographic methods – (paper, TLC and Column chromatography) - High performance thin layer chromatography (HPTLC) - Gas chromatography (GSC/ GLC) technique and sample preparations.

Unit 5 **9Hrs**

Gas chromatography, Mass spectroscopy - High pressure liquid chromatography - Ion exchange chromatography - Ion molecular exclusion chromatography - Capillary electrophoresis.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5
CO6	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K6

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Elective 1:

ADVANCES IN NANOBIOTECHNOLOGY

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

To understand the basics and nanobiotechnology

To understand the advanced techniques in the nanobiotechnology

Course Prerequisites:

To have a basic knowledge in nanobiotechnology and drug delivery systems

Course Outcomes (Cos):

CO-1: Be aware with the principle of nanobiotechnology.

CO-2: Acquire the theoretical knowledge on toxicology assays

CO-3: Explain the theoretical principles of nanoparticles in cancer therapy.

CO-4: Evaluate and suggest suitable techniques for drug delivery system

CO5: Summarise the significance of nanoscale & its dimensions, in 3D bio printing

Course Outline:

Unit 1: Principle of Drug Delivery Systems 6 hrs

Modes of drug delivery, Absorption distribution metabolism excretion characteristics of drugs, Controlled drug delivery - site specific drugs, Barriers for drug targeting - passive and active targeting, Strategies for site specific drug delivery.

Unit 2: Toxicity Assays and their Principles 6 hrs

Cell viability, LDH release, ROS production, Morphological observation, Membrane potential, Live/Dead assay, Comet Assay, Cell cycle analysis and Apoptosis detection by flow cytometer

Unit 3: Nanoparticles and Cancer Therapy 6 hrs

Cancer and its types: Mechanisms of progression in Cancer: Cellular trafficking, Cancer invasion, Migration, Angiogensis and Metastasis. Chemotherapy, Immunotherapy, Photodynamic Therapy (PDT), Photothermal Therapy (PTT), Magnetic Hyperthermia (MHT), High Intensity Focused Ultrasound (HIFU).

Unit 4: Targeted Drug Delivery 6 hrs

Classification of targeted drug delivery systems, Bioconjugation, Nanoparticles surface modification - PEGylation, Gold nanoparticles for drug delivery, Magnetic nanoparticles as drug carriers.

Unit 5: 3D Bio -Printing (Three Dimensional Bio-Printing) 6 hrs

Introduction - History, principle and its components, Classification of 3D bio-printing techniques - Extrusion-based bio-printing, Droplet-based bio-printing, Laser-based bio-printing, Design Requirements for 3D Bio-printing- Magnetic Resonance Imaging, Computed Tomography, Computer-Aided Design Based Systems, 3D modelling softwares, Bio inks for 3D bio-printing - Applications of 3D Bio-printing and future trends.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

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2. Handbook of Nanomaterials for Cancer Theranostics. Conde, J. (Ed.). (2018).
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4. 3D Bio-printing -Fundamentals, Principles and Applications, Ibrahim T. Ozbolat, Academic Press, (2016).
5. 3D Bio-printing in Regenerative Engineering, Principles and Applications, Ali
6. Khademhosseini, Gulden Camci-Unal, 1st edition, CRC press, (2018).

SCIENTIFIC RESEARCH METHODOLOGY

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

Understand the basic needs for literature survey and paper writing.

Understand the instrumental techniques

Course Prerequisites:

The pre-requisite for studying the course is the basic knowledge in research.

Course Outcomes (Cos):

CO-1: Be aware with literature survey.

CO-2: Acquire knowledge about the collection of abstract and searching of abstracts

CO-3: Explain the process of choosing a research problem.

CO-4: Evaluate the instrumental techniques

CO5: summarise the computer technology for literature survey and analysis

Unit 1: Literature Survey 6 hrs

Source of chemical information – primary, secondary, tertiary sources-literature survey-Indexes and abstracts in science and technology – Applied science and technology index, chemical abstracts, chemical titles, current chemical reactions, current contents and science citation index. Classical and comprehensive reference works in chemistry-synthetic methods and techniques, treatises, reviews, patents and monographs.

Unit 2: Chemical Abstracts 6 hrs

Current awareness searching: CA weekly issues, CA issue indexes. Retrospective searching: CA volume indexes-general subject index, chemical substance index-formula index, index of ring systems, author index, patent index. CA collective indexes: collective index (CI), decennial index (DI). Access points for searching CA indexes- Index guide, general subject, terms, chemical substance names, molecular formulas, ring systems, author names, patent numbers. Locating the reference: finding the abstract, finding the original document chemical abstract - service source index.

Unit 3: Choosing a Research Problem and Scientific Writing 6 hrs

Identification of research problem – assessing the status of the problem - guidance from the supervisor – actual investigation and analysis of experimental results – conclusions.

Scientific writing-research reports, thesis, journal articles and books.

Steps to publishing a scientific article in a journal – types of publications-communications, articles, reviews, when to publish, where to publish, specific format required for submission.

Documenting- Abstracts-indicative (or) descriptive abstracts, informative abstract, footnotes, end notes, referencing styles-bibliography-journal abbreviations (CASSI), abbreviation used in scientific writing.

Unit 4: Instrumental Characterization and Data Analysis 6 hrs

Principle and Sample preparation of UV, FT-IR, TEM, SEM, EDAX, AFM and XRD characterization of observed results – Data analysis - Report.

Errors in chemical analysis – classification of errors – determination of accuracy of methods – improving accuracy of analysis – significant figures – mean, standard deviation – comparison of results : "t" test, "f" test, Q test and "chi" square test – rejection of results – presentation of data.

Unit 5: Computer Searches and Literature 6 hrs

ASAP – Alerts, CA Alerts, scifinder, chemport, science direct, STN international, journal home pages. Online browsing of research articles – online submission of research papers in various Journals (ACS, RSC, Elsevier, Springer etc.) –Instructions to the authors – Impact factors. Writing project proposal to funding agencies (UGC, DST etc.).

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

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13. www.ugc.ac.in/pdfnews/7716504_12th-plan-guidelines.pdf
14. R.M. Silverstein, G.C. Bassler and Morril, Spectrometric identification of organic compounds.
15. D.L.Pavia, G.M.Lampman and G.S.Kniz Jr., Introduction to spectroscopy – A guide for students of organic chemistry.
16. H.Willard, L.MerritJr.andA.Dean, Instrumental methods of analysis.
17. D.A.Skoog and M.West, Principles of instrumental analysis.
18. B.K.Sharma, Instrumental methods of chemical analysis
19. D.A. Skoog and M.West, Fundamentals of analytical chemistry.
20. J.D.Dick, Analytical chemistry.
21. S.M.Khopkar, Basic concepts of analytical chemistry.

GREEN CHEMISTRY

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

To understand the principles of green chemistry and environment

To understand the advanced catalytic process

Course Prerequisites:

The pre-requisite for studying the course on Green Chemistry is to have basic information about environment and precaution in using the chemicals.

Course Outcomes (Cos):

CO-1: To remember the green chemical principles and the environment.

CO-2: Understand the use of green chemistry in sustainable development

CO-3: Apply the advances in catalytic process.

CO-4: Analyse the application of catalysis in pharmaceutical industry

CO5: Evaluate the electrochemical and fuel cell technology

Unit 1: Green chemistry and the Environment 6 hrs

Introduction – Green chemistry and industry – Waste minimization and atom Economy – Reduction of materials use – Reduction of energy requirement – Reduction of risk and hazard – Chemistry of the atmosphere – Chemistry of the terrestrial environment – Chemistry of the oceans.

Unit 2: Green chemistry and Sustainable development 6 hrs

The concept of sustainability – The LCA Methodology and applications – Concepts in Acidity and solid acid catalysts – Industrial applications of solid acid catalysts – Some recent developments in catalytic materials and processes – Structured Mesoporous Materials – Catalytic applications – Polymeric tools for organic synthesis – Copolymerisation with usual monomers – Chlorofluropolymers.

Unit 3: Advances in catalysis processes 6 hrs

Chemical production by biocatalysis – Green biocatalytic processes – Nucleophilic aliphatic and aromatic substitutions – Phase transfer combined with metal catalysis – Peroxygen systems and their reactivity – Developments in catalysed oxidations for chemical synthesis – Developments in catalysed oxidations for effluent treatment.

Unit 4: Pharmaceutical Catalysts for Industry and Photochemistry 6 hrs

Focus of process chemistry – Envirocats – Commercial applications of envirocats – Process indensification for green chemistry – Microreactors – Sonochemistry – Ultrasound in electrochemistry – Ultrasound in environmental protection and waste control – Photochemistry – Specialized photochemical reactors and process technology – Photochemical reactors.

Unit 5: Electrochemistry and Fuel Cell Technology 6 hrs

Introduction - Electrochemistry fundamentals – Electrochemistry and energy sustainability – Electrochemical Synthesis – Electrochemistry waste minimization - Fuel cell electrochemistry – Fuel cell technology – Fuel cell applications – Extraction of natural products with superheated water – Properties of superheated water - Chromatography with superheated water.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

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2. Anastas, P. and Zimmerman, J.2003.Design Through the 12 principles of Green Engineering. Environ. Sci.Technol.(37)5:94A-101A.
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SECOND SEMESTER

Core -4: SYNTHESIS OF NANOMATERIALS

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

To learn about bulk synthesis of nanomaterials.

1. To know about physical chemical and biological approaches of nanomaterials synthesis.
2. To understand the lithographic process for the fabrication nanodevices.

Course Prerequisites:

Basic knowledge in synthesis methods of various nanomaterials

Course Outcomes(Cos):

CO1: Understand the basic and advanced concepts of nanomaterial preparations.

CO2: Understand the importance of synthesis method addressed in the material properties and investigate the various factors influencing the properties of nanomaterials.

CO3: Gain expertise in optimizing the synthesis methodology and will be able to fabricate device architectures and new nanomaterials with novel biological activity.

CO4: Illustrate the Synthesis of nanomaterials by biological methods.

CO5: Methods for the fabrication through lithography techniques.

Course Outline:

UNIT I **6Hrs**

Synthesis of bulk nanostructured materials - Sol Gel processing- Mechanical alloying and high energy ball milling-types of balls – WC and ZrO_2 materials – melt quenching and annealing – Etching – Wet cleaning – CMP – Inert gas condensation

UNIT II **12Hrs**

Self-Assembled Monolayers (SAM) - Vapour Liquid Solid (VLS) approach- Chemical Vapour Deposition (CVD) - Langmuir-Blodgett (LB) films - Spin coating - Electrochemical approaches: Anodic oxidation of alumina films, porous silicon and pulsed electrochemical deposition - Spray pyrolysis - Flame pyrolysis - Thin films - Lithography.

UNIT III **9Hrs**

Biological Methods: Biomineralization, biological production of nanoparticles – Phytosynthesis, phycosynthesis, mycosynthesis and Herbal synthesis - bioproduct mediated synthesis of nanoparticles.

UNIT IV **9Hrs**

Evaporation-condensation - Vapour- liquid - solid (VLS) - VLS model - Nucleation and growth - surface and bulk diffusion – kinetics – growth of various nanowires –control of size –precursors and catalysts - single- and multi- wall CNT - Si nanowires – density and diameter – doping in nanowires.

UNIT V **6Hrs**

Lithographical techniques - Physical vapour deposition techniques (Reactive sputtering (DC and RF), laser ablation); Epitaxy-different types of Epitaxy - Lattice mismatch - Liquid Phase Epitaxy (LPE) - Molecular Beam Epitaxy (MBE)- Pulsed laser deposition (PLD) - Atomic layer deposition (ALD).

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K1
CO2	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K2
CO3	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K3
CO4	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K4
CO5	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K5

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Practical – 3: SYNTHESIS OF NANOMATERIALS

L	T	P	C
-	-	3	2

1. Synthesis of Silver Nanoparticles by Chemical reduction method and optical property studies by UV-vis absorption spectroscopy.
2. Synthesis of Gold Nanoparticles by Chemical reduction method and optical property studies by UV-Vis absorption spectroscopy.
3. Preparation of quantum dots such as cadmium selenides and its optical studies.
4. Preparation of cadmium sulphide nanoclusters and its spectral studies.
5. Biosynthesis of Silver Nanoparticles Antibacterial studies of silver nanoparticles by MIC method.
6. Synthesis of thin film by Sol-Gel method
7. Synthesis of metal oxide nanoparticles by microemulsion technique
8. Sol gel synthesis of ZnO nanoparticles

Core – 5: STRUCTURE AND BONDING

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

To provide knowledge of basic and advanced concepts in bonding and enable the students to identify the structure and bonding of simple molecules.

1. To provide an understanding of the various types of solid state packing and the types of chemical forces
2. To enable students appreciate the structure of inorganic chain and cluster compounds.
3. To provide knowledge of the structure and bonding in boron compounds.

Course Pre-requisite:

Basic knowledge in inorganic chemistry

Course outcomes (COs):

At the end of the course, the student will be able to

CO-1: Understand the fundamentals and applications of VSEPR, VBT, and MO theories governing the inorganic chemistry.

CO-2: Analyse the structure and defects of solids.

CO3: Compare and solve the structures, bonding and properties of electron-deficient clusters and cages of Borone, S-N, P-N of inorganic rings, cages, clusters and polymers.

CO4: Realize the fundamentals of solid-state chemistry.

CO-5: Categorize inorganic solids into different classes based on its structure, chemical property, and applications.

Course Outline:

UNIT I: Chemical bonding **9Hrs**

V.B. approach to bonding-Hitler-London, Pauling and Slater refinements, Concept of hybridization and structure of molecules, VSEPR theory shapes of molecules. M.O. approach to covalent bonding – symmetry and overlap of atomic orbitals – symmetry of molecular orbitals – sigma and pi bonding – energy levels in homo and hetero nuclear diatomic systems – bond length, bond order and bond energy, Application to small molecules such as $BeCl_2$, BCl_3 and CCl_4, SF_4, etc, ionic character in a covalent bond - The concept of multicentre bonding. Pseudo halogens: Structure and bonding in ClF_3, BrF_3 , BrF_5 , IF_5, IF_7 etc . Oxides and oxyacids of halogens, Bonding in Noble gas compounds – $XeCl_2$, XeF_4, $XeOF_4$, XeF_6.

UNIT II: Chemistry of solid state I: structure **9Hrs**

Weak Chemical forces: van der Waals forces, Hydrogen bonding, Close packing of atoms and ions HCP and BCC types of packing voids, radius ratio – derivation – its influence on structures. Lattice energy – Born-Lande equation - Kapuscinski equation, Madelung constant.

Representative structures of AB and AB2 types of compounds - rock salt, cesium chloride, wurtzite, zinc blende, rutile, fluorite, antifluorite, cadmium iodide and nickel arsenide. Structure of graphite and diamond. Spinels -normal and inverse types and perovskite structures.

UNIT III: Chemistry of solid state II: diffraction methods **9Hrs**

Band theory of solids- non-stoichiometry- point defects – linear defects- effects due to dislocations- electrical properties of solids-conductor, insulator, semiconductor-intrinsic-impurity semiconductors- optical properties-lasers and phosphors-elementary study of liquid crystals.

Difference between point group and space group – screw axis – glide plane - symmetry elements – relationship between molecular symmetry and crystallographic symmetry – The Concept of reciprocal lattice – X-ray diffraction by single crystal – rotating crystal – powder diffraction. Neutron diffraction: Elementary treatment – comparison with X-ray diffraction. Electron diffraction- Basic principle. Crystal Growth methods: From melt and solution (hydrothermal, Gel methods).

UNIT IV: Boroncompounds and clusters 9Hrs

Chemistry of boron – boranes, higher boranes, borazines , boron nitrides, hydroborate ions – Preparation, properties and structure, STYX numbers, Wade's rules.

Carboranes- Types such as nido-closo, arachno-preaprtion properties and Structure. Metallocarboranes-a general study. Metal clusters: Chemistry of low molecularity metal clusters only, Structure of Re2Cl8; multiple metal-metal bonds.

UNIT V: Inorganic chain and cluster compounds 9Hrs

Types of inorganic polymers, comparison with organic polymers, silanes, higher silanes, multiple bonded systems, silicon nitrides, siloxanes. P-N compounds, cyclophosphazenes and cyclophosphazanes. S-N compounds – S_4N_4, (SN)x.

Isopoly and heteropoly acids – Structure and bonding of 6- and 12 – isopoly and heteropoly anions. Structure of silicates - applications of Paulings rule of electrovalence - isomorphous replacements in silicates – ortho, meta and pyro silicates – one dimensional, two dimensional and three dimensional silicates.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

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2. A.G. Sharpe, Inorganic Chemistry, Pearson Education, 2008.
3. N. H. Ray, Inorganic Polymers, Academic Press, 1978.
4. A. R. West, Basic Solid State Chemistry, John Wiley, 1991.
5. E. L. Mutteri, Polyhedral Boranes, Academic Press, NY, 1975
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7. M. C. Day, J. Selbin, Theoretical Inorganic Chemistry, 2nd Ed, East West Press, 1985.
8. L. Pauling, The Nature of the Chemical Bond, 3rd Ed., Cornell University Press, 1960.
9. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4th Ed, John Wiley & Sons, 1986.

Core – 6: QUANTUM CHEMISTRY AND ANALYTICAL TECHNIQUES

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. To learn the principles of quantum mechanics of simple systems.
2. To learn the quantum mechanical treatment of multi electron atoms.
3. To learn the principles, instrumentation, interpretation and applications of micro wave, IR and Raman spectroscopy.
4. To learn the principles, instrumentation and applications of Polarography, Amperometry, Coulometry
5. To understand the principles, instrumentation and applications of various thermal analysis techniques
6. To understand the principles, instrumentation and applications of various elemental analysis and surface analysis techniques

Course Prerequisites:

Degree level – quantum chemistry and analytical techniques

Course outcomes (COs)

At the end of the course, the student will be able to

CO-1: Recognize the role of multidisciplinary streams especially basic physics & mathematics knowledge in the development of quantum chemistry & thermodynamics

CO-2: Apply the fundamental knowledge in quantum chemistry & thermodynamics to an existing and emerging problem in basic science

CO-3: Understand the basic principles of light-matter interactions and learn quantum mechanical methods to analyze the interactions

CO-4: Apply selection rules in microwave, infrared, Raman, UV-Vis spectroscopy/ Rotational, Vibrational & Electronic spectroscopy

CO-5: Demonstrate the ability to do some independent calculation and use some computational resources at the end of the course Interpretation the spectra of various thermal analysis curves.

CO6: Develop knowledge on working principles of various analytical techniques available for chemical analysis in laboratories

Course outline:

UNIT-I: Quantum chemistry-I **9Hrs**

Black body radiation-Planck's quantum theory-Wave particle duality-Uncertainty Principle. Operators-linear, commutation, Hermitian and Hamiltonian operators. Eigen functions and Eigen values-Postulates of quantum mechanics. Derivation of Schrodinger's time-independent wave equation and its application to particle in a one dimensional box, particle in a three dimensional box, harmonic oscillator, rigid rotor and hydrogen atom.

UNIT-II: Quantum chemistry-II **9Hrs**

Born-Oppenheimer approximation-Hydrogen molecule ion. LCAO-MO and VB treatments of the hydrogen molecule.Antisymmetry and Pauli's exclusion principle. Slater detrimental wave function, term symbols and spectroscopic states-Russell Saunders coupling.

The variation theorem and Perturbation theory. Applications of variation method and perturbation theory to the helium atom. Hybridization-determination of bond angles of sp, sp2 and sp3 hybridizations. Huckel pi electron (HMO) theory and its applications to ethylene, butadiene and benzene. A brief idea of Hartree and Hartree-Fockself consistent field theory.

UNIT III: Rotational and vibrational spectroscopy **9Hrs**

Micro wave spectroscopy- Theory- selection rules, –Instrumentation; Energy levels in atoms and molecules- Fourier transformation Rotational spectra of diatomic and polyatomic molecules–P,Q,R branches- effect of isotopic substitution. Non-rigid rotator- Linear molecules.Theory of Rotational Raman spectra.

Vibrational spectra of diatomic molecules – – selection rules –overtones, combination and hot bands - Fermi resonance Energy of diatomic molecule, simple harmonic and unharmonic oscillator, rotational character of vibration spectra, Theory of Vibrational Raman spectroscopy-Coherant Antistokes Raman Spectroscopy (CARS).

UNIT IV: Analytical techniques 9Hrs

Principles, theory, instrumentation and applications of Polarography, amperometry, coulometry, XRD, EDAX, XPS, AAS, AES, interpretation of spectra-Merits and demerits.

UNIT V: Surface and thermal analysis techniques 9Hrs

Principles, theory, instrumentation and applications of SEM, STM, TEM, AFM, ESCA - interpretation of spectra-Merits and demerits.

Principles, theory and applications of TGA, DTA, DSC, DTG. Interpretation of various thermal analysis curves.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K1
CO2	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K2
CO3	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K3
CO4	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K4
CO5	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K5
CO6	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K6

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1. R. K. Prasad, Quantum Chemistry, Wiley Eastern, 1993.
2. C. F. Banwell, Fundamentals of Molecular Spectroscopy, McGraw Hill, New York, 1966.
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10. M. W. Hanna, Quantum Mechanics in Chemistry, W. A Benjamin Inc. London 1965.
11. I. N. Levine, Quantum Chemistry, Allyn and Bacon, Boston, 1983.
12. H. Eyring, J. Walter and G. Kimball, Quantum Chemistry, John Wiley and Sons, New York, 1944.
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15. D. A. McQuarrie, Quantum Chemistry, University Science Books, MilValley, California, 1998.
16. B. K. Sen, Quantum Chemistry, Tata McGraw Hill, 1992.
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18. W. Levine, Quantum Chemistry, Prentice Hall, 1994.

Practical – 4: STRUCTURE AND BONDING AND QUANTUM CHEMISTRY AND ANALYTICAL TECHNIQUES

L	T	P	C
-	-	3	2

Practical – 4: STRUCTURE AND BONDING

1. To study rate of equation of 1,10 Phenanthroline Fe(II) in acid solution by spectrophotometry.
2. Synthesis, purification & analysis of co-ordination complexes of simple & chelating ligands. (Any-2)
   i) Bis (acetylacetonato complex of Cu (II), Co(II) & VO (IV) (any – one)
   ii) $[Cr(NH_3)_6]\ Cl_3$
   iii) $[Ti\ (urea)_6]I_3$
   iv) Salicyladoxime (Fe or Cu)
   v) Prussion – blue $Fe_4\ [Fe(CN)_6\ ]_3$
3. Determination of dissociation constant of an acid - base indicator by Spectrophotometry method

Practical – 4: QUANTUM CHEMISTRY AND ANALYTICAL TECHNIQUES

1. Determination of solubility diagram for a three component liquid system.
2. Radiolysis of aqueous iodate solution and determination of G values.
3. Molecular weight of a polymer by end group estimation.
4. Determination of the formula of complexes such as silver –ammonia complex by titration, cuprammonium ion complex by distribution coefficient measurement,
5. Determine the transport number of silver and nitrate ions in aqueous solution from the cell potential of the concentration cell with junction potential.
6. Recording of TGA curve of CuSO4 and NaCl and hence to find the percentage composition of the mixture.
7. Determination of the heat of ionization of phenol/weak acid.

Online Course from Swayam, MOOCs, NPTEL etc.

Elective 2:

INDUSTRIAL NANOTECHNOLOGY

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

1. To educate the students on industrial application of nanotechnology
2. To impart understanding of industrial process

Course Prerequisites:

The pre-requisite for studying the course on Industrial Nanotechnology is basic knowledge on the nanoscience and nanotechnology

Course Outcomes (Cos):

At the end of the course the students should able to

CO1: Learn about the semiconductor devices.

CO2: gain knowledge on magnetic materials.

CO3: Aware about optical storage devices.

CO4: Explain the industrial applications of nanotechnology

Course Outline:

Unit 1 **6 hrs**

Semiconductor Nanostructures and devices, Fabrication and Applications of different types of semiconductor Nanostructures- Silicon horizontal and vertical core shell Nanowires- Integrated circuits- Sensors- Electro optical devices.

Unit 2 **6 hrs**

Semiconductor Quantum dots (QDs) – QD LASER- Quantum cascade LASER-QD optical memory- Present and future trends. Nanoscale Magnetic Materials: Application in magnetic storage devices- storing and reading device – current trends of spin based electronic devices.

Unit 3 **4 hrs**

Optical storage devices: Near field optical recording- holographic data storage- AFM based recording technology.

Unit 4 **6 hrs**

Nano Electro Mechanical Systems: Overview- Nano-Electromechanical systems - fabrication process- choice of materials, performance of different structures - advantages and disadvantages of different approaches. Applications in sensors, Micro actuators - Extension to the Nanoscale.

Unit 5 **6 hrs**

Industrial Applications of Nanomaterials: Nanoparticles and Micro –organism, Nano-materials in bone substitutes & Dentistry, Food and Cosmetic applications, Textiles, Paints, Catalysis, Drug delivery and its applications, Biochips- analytical devices, Biosensors.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K1
CO2	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K2
CO3	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K3
CO4	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K4

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APPLIED CHEMISTRY

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

1. To educate the students on the use of chemistry in day to day life
2. To impart understanding on chemistry in life science

Course Prerequisites:

The pre-requisite for studying the course on Applied Chemistry is basic knowledge on the chemical process

Course Outcomes (Cos):

At the end of the course the students should able to

CO1: Learn about the daily usage of chemicals in life.

CO2: gain knowledge on the materials use for food and other basic needs.

Co3: Aware about the pharmaceutical applications of chemistry.

CO4: Explain the role of chemistry in day to day life

Course Outline:

UNIT 1: Soaps and Detergents **5 hrs**

Soaps: Definition-classification-raw materials used in the manufacture of soap –manufacture of toilet soap. Detergents: Definition –various types with examples- advantages of detergents over soaps – cleansing action of soap.

UNIT 2: Fertilizers **5 hrs**

Definition-characteristics of a good fertilizer- role of nitrogen, potassium and phosphorous in plant growth – natural fertilizers- chemical fertilizers: urea, muriate of potash and triple superphosphate - mixed fertilizers – biofertilizers – advantages of biofertilizers.

UNIT 3: Polymers **6 hrs**

Fibers: Classification –uses of terylene, nylon and orlon. Resins: Natural resins- synthetic resins-type-uses of fevicol, quick fix, araldite, glyptal and Bakelite. Plastics: classification- differences between thermoplasts and thermosets. Advantages of plastics-uses of polythene, PVC, polystyrene, Teflon and thermocole. Rubber: Types-defects in natural rubber-vulcanization-synthetic rubbers-uses of neoprene, thiocol, butyl rubber, silicone rubber and foam rubber.

UNIT 4: Chemicals in Pharmacy 5 hrs

Definition and therapeutic uses of the following (an elementary study only) Antiseptics: alum, boric acid Mouth washes: Hydrogen peroxide Antacids: Aluminium hydroxide Analgesics: Aspirin, paracetamol Antibiotics: Penicillins, tetracyclines Haematinics: Ferrous fumerate, ferrous gluconate Laxatives: Epsom salt, milk of magnesia Sedatives: Diazepam

UNIT 5: Chemicals in Day-to-Day Life 4 hrs

An outline of the preparation and uses of the following articles. Tooth powder, tooth paste, writing inks, gum paste, boot polish, talcum powder, chalk crayons, agar battis, phenyl and moth balls.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	K1
CO2	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	K2
CO3	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	K3
CO4	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	M	K4

References

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IPR AND BIOSAFETY

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

1. To educate the students on industrial property rights
2. To impart understanding on patents and biosafety

Course Prerequisites:

The pre-requisite for studying the course on IPR and Biosafety is basic knowledge on the research activities

Course Outcomes (Cos):

At the end of the course the students should able to

CO1: Remember the concepts of IPR.

CO2: Understand the patents and their importance.

CO3: Apply the concept of biosafety in research methodologies.

CO4: Analyse the rules of biosafety

Course Outline:

Unit 1: Types of IP **6 hrs**

Patents – Trademarks - Copyright & Related Rights - Industrial Design - Traditional knowledge- Geographical indications - Protection of new GMOs; International framework for the protection of IP - Invention in context of ―prior art‖ - Patent databases - Searching International Databases - Country-wise patent searches (USPTO, EPO, India etc.) - Analysis and report formation.

Unit 2: Types of Patents **6 hrs**

Indian patent act 1970 - Recent amendments - Patent application- forms and guidelines –Fee structure -Time frames - Filing of a patent application - Precautions before patenting disclosure/non-disclosure - Patent application- Forms and guidelines -Fee structure –Time frames - Types of patent applications -Provisional and complete specifications - PCT and convention patent applications - International patenting – Requirement -Procedures and costs - Financial assistance for patenting-introduction to existing schemes.

Unit 3: IPR Policies **6 hrs**

IPR policy of Government of India - Indian &international patent laws - Indian patent act 1970; recent amendments - Financial assistance for patenting-existing schemes- Role of patents in biotechnology - The patentability of microorganisms - IPR and WTO regime – consumer protection and plant genetic resources-GATT and TRIPS - Patenting gene - Issues and case studies.

Unit 4: Biosafety **6 hrs**

Historical background - Introduction to biological safety cabinets - Primary containment for biohazards - Biosafety levels- Biosafety levels of specific microorganisms - Recommended

biosafety levels for infectious agents and infected animals - Biosafety guidelines – Government of India.

Unit 5: Rules in Biosafety and Contemporary Issues 6 hrs

Definition of GMOs & LMOs - Roles of institutional biosafety committee - RCGM, GEAC - GMO applications in food and agriculture - Environmental release of GMOs - Risk analysis - Risk assessment - Risk management and communication - Overview of national regulations and relevant international agreements including Cartagena protocol-Expert lectures, online seminars – webinars

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K1
CO2	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K2
CO3	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K3
CO4	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K4

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8. Wooley; Karen B. Byers, ASM Press, Washington, DC, USA, 2017.

FIELD WORK

THIRD SEMESTER

Core – 7: REACTION MECHANISM, REARRANGEMENT, NAME REACTIONS, OXIDATION AND REDUCTION

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. Understanding addition and elimination reactions along with their mechanism and synthetic utility.
2. Understanding rearrangement and name reactions along with their mechanism and synthetic utility.
3. Understanding various types of oxidation and reduction reactions along with their mechanism and synthetic utility.

Course Pre-requisite

This core course designed for the students who have acquired basic knowledge of reaction mechanisms.

Course outcomes (COs):

At the end of the course, the student will be able to

CO1: Understanding the basic concepts about how the organic reactions are carried out and also to make the students understand the mechanisms of different organic reactions including various stereochemical, mechanistic and conformational aspects

CO2: Interpret and distinguish reaction mechanism of various addition reactions

CO3: Determine the mechanism for elimination reactions

CO4: explain the mechanism of molecular rearrangement reaction.

CO5: Apply the basic oxidation and reduction reactions on organic molecules.

CO6: Plan to develop and modify the synthesize molecules using popularly named reactions.

Course outline:

UNIT I: Addition to carbon-carbon double bond 9Hrs

Electrophilic addition to carbon–carbon double and triple bonds. Nucleophilic addition to carbon–carbon multiple bonds. Generation and addition of carbenes-Michael addition and Robinson annulation.

Hydroxylation of olefinic double bonds (OsO4, KMnO4); Woodward and Prevost oxidation. Epoxidation using peracids including Sharpless epoxidation, Ozonolysis. Hydrogenation (homogenous and heterogeneous) and Transfer hydrogenation. Hydration of carbon-carbon double and triple bonds.

UNIT II: Addition to carbon-oxygen double bond 9Hrs

Nucleophilic addition to –C=O bond. A study of Mannich, benzoin, Darzen's glycidic ester, Stobbe and Knovenagel condensation reactions; Wittig, Wittig-Horner olefination reactions; Sulfur and Sulfonium ylides and their reactions, Julia olefination & Peterson alkene synthesis. Asymmetric reduction of carbonyl functions (Corey's procedure).

UNIT III: Elimination 9Hrs

Elimination reactions: E1, E2, E1cb and Ei-elimination. Conformation of mechanism; solvent, substrate, leaving group effects-Saytzeff's Vs Hoffman elimination; Stereochemistry of E2 eliminations, Elimination in cyclohexane ring system; Mechanism of pyrolytic eliminations. Examples: Chugaev reactions and Cope elimination, Hoffmann degradation and pyrolysis of esters.

UNIT IV: Molecular rearrangments & name reactions 9Hrs

A study of mechanism of the following rearrangements: Beckmann, Curtius, Hofmann, Schmidt, Lossen, Wolff, Pinacol, Wagner Meerwin, Demjanov, Dienone-Phenol, Favorski, Benzidine, Claisen, Cope, Sommlet-Hauser, Pummerer and Von-Richter rearrangements.

A study of the following name reactions: Dieckmann cyclization, Hofmann-Loffler Freytag reaction, Mitsunobu reaction, Shapiro reaction, Eschenmoser-Tanabe and Ramburg-Backlund reactions.

UNIT V: Oxidation and reductions reactions 9Hrs

Oxidation with Cr (including PCC, PDC, Jones) and Mn (including MnO_2 and $BaMnO_4$) reagents; Oxidation with LTA, DDQ and SeO_2; Oxidation using DMSO either with DCC or Ac_2O or Oxaloyl chloride; Oxidation using IBX and Dess-Martin Periodinane (DMP) reagent.

Reduction with $NaBH_4$, $NaCNBH_3$, $Zn(BH_4)_2$ $LiAlH_4$, $Li(tBuO)_3AlH$, DIBAL-H, Red-Al, Et_3SiH and Bu3SnH; Reduction using selectrides; Birch reduction.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K6

References

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Practical -5: REACTION MECHANISM, REARRANGEMENT, NAME REACTIONS, OXIDATION AND REDUCTION

L	T	P	C
-	-	3	2

1. Preparation of benzanilide by Beckmann rearrangement

2. Preparation of p- Amino benzoic acid
3. Preparation of p- chloro nitrobenzene by Sandmeyer reaction
4. Preparation of p- Iodonitrobenzene by Sandmeyer reaction
5. Pinacol- Pinacolone rearrangement
6. Aldol condensation: Dibenzal acetone from Benzaldehyde
7. Knoevenagel condensation reaction

Core – 8: COORDINATION CHEMISTRY

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. To learn about thermodynamic and stereochemical aspects of complex formation
2. To learn about Various theories of complexes and their magnetic properties
3. To learn about term symbols and energy level diagram of weak and strong field ligands, charge transfer spectra and spectral properties of lanthanides and actinides.
4. To learn about various mechanisms of substitution and electron transfer reactions.
5. To study the recent development in the catalysis

Course Prerequisites:

Knowledge in basics in coordination chemistry

Course outcomes

At the end of the course, the student will be able to

CO-1: Understand the basics of coordination chemistry including coordination numbers, geometry, and chelate effect. Study the bonding theories VBT, CFT, and MOT in turn describe CFSE, High and low spin complexes, magnetic moment of coordination compounds

CO-2: Interpret the electronic spectra of coordination compounds explaining color, allowed and forbidden transitions through Orgel and Tanabe-Sugano diagrams.

CO-3: Design reaction mechanism pathways like associative/dissociative, inner and outer sphere mechanism including electron transfer pathways.

CO-4: Demonstrate the basics, spectral and magnetic properties of Lanthanides and Actinides.

CO-5: Devise special reactions of organometallic chemistry: Oxidative addition, reductive elimination and migratory insertion.

CO-6: Design the catalytic cycles, mechanistic studies and apply metal-catalyzed reactions for industrial applications.

Course Outline:

UNIT I: Stability of complexes 9Hrs

Stability of complexes- Factors affecting stability of complexes, Thermodynamic aspects of complex formation, Stepwise and overall formation constants, Stability correlations, statistical factors and chelate effect, Determination of stability constant and composition of the complexes: Formation curves and Bjerrum's half method,Potentiometric method, Spectrophotometric method, Ion exchange method, Polorographic method and Continuous variation method (Job's method).

Stereochemical aspects- Stereoisomerism in inorganic complexes- Isomerism arising out of ligand distribution and ligand conformation, Chirality and nomenclature of chiral complexes; Application of ORD and CD in the identification of complexes.

Macrocyclic ligands- Porphyrins, Corrins, Schiff's bases, crown ethers, etc.

UNIT II: Metal Ligand Bonding 9Hrs

Crystal field theory – Splitting of d orbitals under various geometries - factors affecting splitting, CFSE, evidences for CFSE (Structural and thermodynamic effects), spectrochemical series, Jorgensen relation, site preferences, Jahn Teller distortion – Dynamic and Static J.T. effect, Jahn Teller effect and chelation, Application of CFT – Magnetic properties, spectral properties and Kinetic properties, Limitations of CFT, Evidences for M-L overlap.

MOT – MO theory and energy level diagrams concept of Weak and strong fields, Sigma and pi bonding in octahedral, square planar and tetrahedral complexes. Nephlauxetic effect, Magnetic properties of complexes. Comparison of CFT and MOT of bonding in octahedral complexes.

UNIT-III: Electronic spectra of complexes 9Hrs

Spectroscopic term symbols for d^n ions – derivation of term symbols and ground state term symbol, Hund's rule, Selection rules – breakdown of selection rules, spin orbit coupling, band intensities, weak and strong field limits – correlation diagram, Energy level diagrams. Orgel diagram for weak field Oh and Td complexes – Splitting of energy level due to Jahn-Teller distortion. Modified orgel diagram – Limitations of orgel diagram Tanabe–Sugano (T-S) diagrams – Evaluation of Dq and B values for d^2 –d^8 complexes charge transfer spectra. Complications in band classification between Lf(d-d) and CT bands. Comparison between d-d bands and CT bands – Numerical problems, Lanthanides and Actinides- Spectral properties.

UNIT IV: Inorganic reaction mechanism 9Hrs

Electron transfer reactions – Inner sphere (ISET) and outer sphere (OSET) electron transfer processes.. Role of bridging ligand with ISET reaction – tunneling transfer – multiple bridging in the

activated complex in the ISET process. Complimentary and non-complimentary ET reactions. Cross reactions and marcus Hush theory.

Reaction mechanism of coordination compounds – Types of ligand substitution reactions – mechanism; Dissociative mechanism (D), Associative mechanism (A) interchanges mechanism (I), Labile and Inert complexes. Substitution Reaction in octahedral complexes – general mechanism, general rate law for A,D and I - distinction between D, Id, IA pathways, replacement of coordinated water, mechanism of acid hydrolysis, base hydrolysis – DCB mechanism – direct and indirect evidences in favour of the mechanism. Ligand substitution reactions without cleavage of M-L Bond. Anation Reactions. Substituion in square planar complexes – General mechanism, Trans effect, influences of entering and leaving groups. Application of trans effect – synthesis of isomers of pt(II) complexes – theories of trans effect and cis-trans isomerisation reaction. Application of substitution reactions in the synthesis of Platinum and Cobalt complexes.

UNIT-V: Catalysis **9Hrs**

General principles of catalysis – basic reactions involved in the catalysis by organometallic compounds. Hydrogenation of olefins (Wilkinson's catalyst); Hydro formylation of olefins using Cobalt or Rhodium catalysts (OXO process); oxidation of olefins to aldehydes and ketones (wacker process) Monsanto acetic acid synthesis from methanol. Cyclooligomerisation of acetylene using Ni catalyst (Reppe's catalyst) Synthetic gasoline by using ZSM-5 catalyst (Fisher-Tropsch and mobil process) polymerization of olefins (Zeigler – Natta Catalyst), polymer bound catalyst.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K6
CO6	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K6

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1. D. Bannerjea, Co-ordination Chemistry, TATA Mcgraw Hill, 1993.
2. M. L. Tobe, Inorganic Reaction Mechanism, Nelson, 1972.
3. K. Burjer, Co-ordination Chemistry Experimental Methods, Butterworths, 1973.
4. B. N. Figgis, Introduction to Ligand Fields, Wiley Eastern Ltd, 1976.
5. W. E. Addision, Structural Principles of Inorganic Chemistry, Longman, 1961.
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7. F. Basolo and R. G. Pearson, Mechanism of Inorganic reactions, Wiley Eastern, 1967.
8. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic chemistry-Principles on structure and reactivity, 4th Ed, Pearson- education, 2002.
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13. R. B. Heslop and K. Jones, Inorganic Chemistry, Elsevier, 1976.

Core – 9: THERMODYNAMICS AND GROUP THEORY

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. To know the limitations of classical thermodynamics in the evaluation of macroscopic properties.
2. To understand the principles of activity and fugacity.
3. To know the theories of kinetic activity.
4. To study the techniques of Heat Capacity.
5. To learn about the various applications of Quantum Statistics.
6. To understand the concepts of group theory
7. To apply group theory for determining vibrations, hybrid orbitals
8. To determine the selection rules for spectral transitions, energies and molecular orbitals

Course Pre-requisite

Degree level knowledge in thermodynamics and group theory

Course outcomes(COs)

At the end of the course, the student will be able to

CO-1: Understand the basic concepts of symmetry and its mathematical expression.

CO-2: Apply these mathematical notations into objects and molecules.

CO-3: Analyze infrared, Raman, and electronic spectra of simple molecules.

CO-4: Identify the need and fundamental derivation of statistical thermodynamics.

CO-5: Summarise the fundamentals of group theory. Explain the orbital symmetry and energy levels and in the conjugated alkenes.

CO-6: Apply group theory and construct the character table to analyse the molecular properties

Course Outline:

UNIT-I: Thermodynamics and Non-ideal systems 9Hrs

Concepts of Partial Molar Properties-Partial Molar Free Energy and Partial Molar Volume.Gibbs-Duhem equation, Chemical potential-Variation of chemical potential with temperature and pressure, Van't Hoff isotherm. Fugacity–Determination of fugacity of gases by graphical method-Variation of fugacity with temperature and pressure -Lewis Randal rule-Duhem-Margules equation. Determination of activity and activity coefficient of non-electrolyte (e.m.f method)-Excess functions.

UNIT-II: Irreversible Thermodynamics 9Hrs

Nernst heat theorem-Third law of thermodynamics-Applications of third law-Entropy change-Calculation of absolute entropies-Apparent exceptions to third law- Non-equilibrium thermodynamics-Basic concepts-Forces and fluxes-Entropy of irreversible processes-Entropy production-Clausius inequality-Phenomenological equations-Onsager reciprocity relations-Coupled reactions. The principal of microscopic reversibility, the Onsager reciprocal relations – verification. Entropy production- rate of entropy production, entropy production in chemical reactions.

UNIT-III: Statistical Thermodynamics 9Hrs

Objectives of statistical thermodynamics, Concept of distributions, Types of ensembles. Thermodynamic probability, Most probable distribution Law- Classical statistics-Maxwell-Boltzmann (MB) statistics-Quantum statistics-Bose-Einstein (BE) and Fermi-Dirac (FD) statistics-Derivation of distribution function-MB, BE and FD statistics-comparison-Partition functions-Translational, rotational, vibrational and electronic partition function –Calculation of thermodynamic parameters and equilibrium constants in terms of partition function; Debye and Einstein heat capacity of solids.

UNIT IV: Group Theory-I 9Hrs

Symmetry elements; symmetry operations, Abelian group-point groups-determination of point group- Group multiplication table - Matrix representation of symmetry operations-Similarity transformations; Space groups of crystals-Mulliken symbols-reducible and irreducible representations; Symbols and rules of irreducible representations-reduction formula-direct product representation; Great orthogonality theorem; character table-construction of character tables C_2v, C_3v and D_2h.

UNIT V: Group Theory-II **9Hrs**

Applications of group theory- Determination of representations of vibrational modes in non-linear molecules such as water, ammonia, BF_3, CH_4 and XeF_4.Determination of Hybrid orbitals in non-linear molecules – Examples: H_2O, NH_3, BF_3, CH_4 and XeF_4. SALC procedure-evaluation of energies and molecular orbitals for systems like ethylene and butadiene.Selection rules for spectral transitions. Electronic spectra of formaldehyde and ethylene.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K1
CO2	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K2
CO3	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K3
CO4	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K4
CO5	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K3,K5

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12. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, New Delhi, 1960.

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Practical – 6: COORDINATION CHEMISTRY AND THERMODYNAMICS AND GROUP THEORY

L	T	P	C
-	-	3	2

CO-1: Understand the safety and precautionary measures in handling chemicals.

CO-2: Synthesize the given list of compounds using standard procedure in a pure form.

Practical -6: COORDINATION CHEMISTRY

1. Preparation of sodium trioxalato ferrate (III), Na_3 Fe $(C_2O_4)_3$ and determination of its composition by permaganometry.
2. Preparation of Ni-DMG complex, Ni $(DMG)_2$.
3. Preparation of copper tetra-amine complex, $Cu(NH_3)_4SO_4$.

4. Preparation of cis-and trans-bisoxalato diaquachromate (III) ion.
5. Analysis of Cu as CuSCN and Ni as Ni (dimethylglyoxime).

Practical -6: THERMODYNAMICS AND GROUP THEORY

1. Determination of the apparent degree of dissociation of an electrolyte (e.g NaCl) in aqueous solution at different concentrations by ebullioscopy.
2. To determine the heat of neutralization of strong acid (HCl, H_2SO_4) and weak acid (acetic acid).
3. Determination of equilibrium constant for the system I_2 +KI KI_3 and to determine the concentration of given KI solution.
4. To verify Beer-Lambert law for $KMnO_4/K_2Cr_2O_7$ and determine the concentration of the given solution of the substance.
5. To study the distribution of benzoic acid between benzene and water.
6. To study the distribution of iodine between carbon tetrachloride and water.
7. To determine the percentage composition of a given mixture (non-interacting systems) by viscosity method.

Elective 3:

INTRODUCTION TO NANOTOXICOLOGY

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

1. To understand the principles of nanotoxicology.
2. To know the nano pollution.

Course Pre-requisite

Degree level knowledge in thermodynamics and group theory

Course outcomes (COs)

At the end of the course, the student will be able to

CO-1: Understand the basic concepts of toxicology.

CO-2: Apply these principles in kinetics of toxicology.

CO-3: Analyze about nanopollution.

CO-4: Identify the human exposure to pollution.

CO-5: Apply the toxicological principles in pollution control

Course Outline:

Unit 1 **4 hrs**

Introduction – Definition of terms-Toxicity-Hazards and hazard types-risk and assessment of risk.

Unit 2 **4 hrs**

Mechanism of Nanosize particle toxicity-Passage through biological membranes-toxicokinetics

Unit 3 **4 hrs**

Nanopollution – Nanomaterials in environment-sources of pollution-transport through environment

Unit 4 **4 hrs**

Human exposure to nanosized materials-measurement-Threshold-permissable limits

Unit 5 **4 hrs**

Portals of entry and target tissue-routes of entry of pollutants-distribution and target tissue.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

References

1. Nanotechnology: Health and Environmental Risks, Jo Anne Shatkin, CRC Press, 2008
2. Nanotechnology: Environmental Health and Safety, Risks, Regulation and Management, Matthew Hull and Diana Bowman, Elsevier, 2010
3. Principles and Methods of Toxicology. Edited by A.W. Hayes. Taylor and Francis, 2008.

COMPUTATIONAL NANOSCIENCE

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

1. To understand the computational activity of nanoscience.
2. To know physics, chemistry and biology of computational nanoscience.

Course Pre-requisite

Degree level knowledge in computational theories

Course outcomes (COs)

At the end of the course, the student will be able to

CO-1: Understand the basic concepts of computational aspects.

CO-2: Apply these in physics, chemistry and biological field.

CO-3: Analyze in the optical and vibrational properties of materials.

CO-4: Identify the molecular dynamics of computational nanoscience.

CO-5: Apply the principles in DNA technology

Course Outline:

Unit 1 **6 hrs**

Introduction: Computational aspects of physics, chemistry and biology- high- performance computers- parallel computing- algorithms- computational complexity- Bio-O notation- P, NP, NP-complete and NP hard algorithms- decision and optimisation problems- examples: travelling salesman problem, Hamiltonian path problem, satisfiability problem.

Unit 2 **6 hrs**

Computational physics: General theory and methods- optical and vibrational properties of materials- mechanical behaviour- multiscale modelling of materials- large- scale simulations- materials at high pressure and high temperature- alloys and nanostructures- semiconductors and electronic materials.

Unit 3 **4 hrs**

Nano grain formation and stability- transport in nanostructures- quantum confined systems- growth aspects of nanotubes- theoretical study of carbon nanotubes- thermal properties of nanostructures-

Unit 4 **6 hrs**

Computational chemistry: General computational chemistry- theory and methods- molecular mechanics- molecular dynamics- theory and applications- combinatorial chemistry- kinetics and collision dynamics- polymers and colloids- solid state and surface chemistry- catalysis, separation and reactions – formulations and QSAR- molecular electronic structure.

Unit 5 **6 hrs**

Computational Biology: Bioinformatics- algorithms in bioinformatics- molecular modelling- structural bioinformatics- algorithms- computational genomics- computational drug/ molecular design- self-replicating/organizing systems. DNA nanotechnology- DNA and protein computers.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

References

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2. Computational Complexity, C.H. Papadimitriou (1994), Addison Wesley, USA
3. Computational methods in physics, chemistry and Biology, P. Harrison (2001), John Wiley and Sons, USA
4. A computational approach to chemistry, D.M. Hirst (1990), Blackwell Scientific Publications, USA
5. Introduction to computational molecular Biology, J. Setubal and J. Meidains (1997), PWS Publishing company, USA
6. Molecular Dynamics Simulations, J.M. Haile (1992), John Wiley and Sons, USA
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8. Computational Neuroscience, J. Feng (2004), Chapman and Hall/CRC, USA.

NANOCOMPOSITE

L	T	P	C
3	-	-	3

Course Code:

Course Objectives:

Understand the bases for the molecular structure and Nanocomposites

To know the principle involved in the separation of Protein-based Nanostructures.

Course Pre-requisite

Degree level knowledge in thermodynamics and group theory

Course outcomes (COs)

At the end of the course, the student will be able to

CO-1: Understand the basic concepts of nanocomposites.

CO-2: Apply the physics of modulus in nanocomposites.

CO-3: Analyze the processing of nanocomposites.

CO-4: Identify the characterization techniques of nanocomposites.

CO-5: Apply the nanocomposites in optical fields

Course Outline:

Unit I **6 hrs**

Introduction of Nanocomposites: Nanocomposites- Definition - Nanocomposites past and present- Nomenclature -Solids -Atomic and molecular solids -Role of statistics in materials -Primary , secondary and tertiary structure - Transitions

Unit II **6 hrs**

Properties and features of nanocomposites: Physics of modulus - Continuum measurements -Yield - Fracture -Rubbery elasticity and viscoelasticity - Composites and nanocomposites -Surface mechanical properties -Diffusion and permeability -Features of nanocomposites -basics of polymer nano compos1tes

Unit III **6 hrs**

Processing of nanocomposites: Viscosity -Types of flow -Viscosity - Experimental viscosity -Non-newtonian Flow -Low-viscosity processing –Solvent processing -Particle behavior -In situ polymerization -Post-Forming -Hazards of solvent Processing -Melt, high -shear, and direct processing

Unit IV **6 hrs**

Characterization of nanocomposites: Introduction to characterization - Experiment design -Sample preparation -Imaging -Structural characterization - Scales in nanocomposites -Texture - Electromagnetic energy -Visualization - Physicochemical analysis -Characterization of physical properties -Identification -\Mechanical -Surface mechanical properties.

Unit V **6 hrs**

Applications of nanocomposites: Nanocomposites -Optical, structural applications -Nanoparticulate systems with organic matrices -Applications - Biodegradable protein nanocomposites -Applications

Polypropylene nanocomposites - Application as exterior automatic components -Hybrid nanocomposite materials - Application for corrosion protection

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5

References

1. Thomas E. Twardow ski, Introduction to Nanocomposite Materials -Properties, Processing, Characterization, DesTech Publications, April 2007

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Online Course from Swayam, MOOCs, NPTEL etc.

MINI PROJECT

FOURTH SEMESTER

Core – 10: PHOTOCHEMISTRY, PERICYCLIC REACTIONS, HETEROCYCLES AND NATURAL PRODUCTS

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. Imparting knowledge in the theory and applications of various aspects of photochemistry and pericyclic reactions.
2. To understand the synthesis and reactivity of five- as well as six-member heterocycles.
3. To understand the structural elucidation, biosynthesis and synthesis of natural products – Terpenoids, Alkaloids & Steroids.

Course Prerequisites

Knowledge in photochemical reactions and synthesis of natural products

Course Outcomes(Cos):

At the end of the course, the student will be able to

CO1: understand the chemistry of vision by fundamental principles of photochemical reactions and also pericyclic reactions, correlation diagrams, rearrangements and related problem.

CO2: the utility of important reagents used in the multistep synthesis of medicinally relevant heterocyclic compounds and the mechanisms involved in each step.

CO3: Demonstrate the steps involved in the structure elucidation of various natural products using chemical, analytical and synthetic methods of alkaloids.

CO4: illustrate the structure, stereochemistry and synthesis of steroids and terpenoids.

CO5: Evaluate the photochemical reactions based on the influence of the substituents on substrate molecules.

CO6: Design new photochemical reactions in order to achieve the required product(s).

Course Outline:

Unit-I: Organic Photochemistry **9Hrs**

Principles of Photochemistry and Photochemical reactions: Norrish type I & II reactions. Paterno-Büchi reaction; Photochemistry of enones and dienones: [2 + 2] photochemical cycloaddition; Photo Fries, di-π methane, oxa & aza di-π methane rearrangements.

Unit II: Orbital Symmetry & Pericyclic Reactions **9Hrs**

Selection rules (Woodward and Hoffmann rules) and stereochemistry of electrocyclic reactions, cycloadditions and Sigmatropic reactions-FMO approach, Correlation diagram approach, Huckel-Mobius approach and perturbation molecular orbital approach.

Unit-III: Heterocycles and Their Reactivity **9Hrs**

Structure, synthesis and their reaction of the following systems; a) One heteroatom -Pyrrole, Furan, Thiophene, Pyridine; b) Benzo fused Heterocycles - Indole, Quinoline; c) Two heteroatom - Pyrazole, Imidazole, Pyrimidine, Pyrazine.

Unit-IV: Natural Products: Terpenoids & Steroids **9Hrs**

Terpenoids: Isolation and classification - general methods to elucidate the structure of terpenoids - methods of structure elucidation and synthesis as applied to zingiberine - eudesmol - caryophyllene - abietic acid - santonin - biosynthesis of terpenes.

Steroids: Structural elucidation of cholesterol – erogosterol- vitamin-D – equilenin – estrone - progesterone, Stigmasterol, Steriod harmones, androsterone, testosterone, biosynthesis of steroids – Structure - Synthesis of bile acids.

Unit-V: Natural Products: Alkaloids **9Hrs**

Structural elucidation and biosynthesis of dictamnine – chinconine – morphine – reserpine – aeronycine – cocaine – lysergic acid and nicotine.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cognitive level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5
CO6	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K6

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Core – 11: INORGANIC PHOTOCHEMISTRY, SPECTROSCOPY AND ORGANOMETALLICS

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. To learn the photo electron spectroscopy of inorganic compounds.
2. To study the theory, determination of structure, growth of crystals.
3. To study the applications of IR, Raman and NMR spectroscopy in inorganic compounds
4. To learn the detail study of synthetic organometallic complexes and their reactivity.
5. To know about ESR and Mössbauer spectroscopy

Course Pre-requisites:

Acquire knowledge inorganic photochemistry, spectroscopy and organometallics

Course outcomes(COs)

At the end of the course the students should able to

CO1: Understanding the inorganic photochemical reactions to evaluate the reaction path and in photochemical energy conversion like solar cell, fuel cell etc.

CO2: Apply the knowledge of radioactivity and nuclear reactions into various applications such as radio-dating, reaction mechanisms, and nuclear energy.

CO3: Outline the basic principles and instrumentation of spectral techniques like IR, Raman, NMR, and electronic spectroscopy and analyse their application in determining the structure and property of Inorganic compound/complexes

CO4: Unravel and interpret the photochemical properties of coordination complexes

CO5: Define the terms EAN, 18, 16-electron rule classify the organometallic compounds, structure and properties of organometallic compounds such as metallocene, alkenes, alkynes and arene complexes.

CO6: determine and evaluate the synthesis, structure and reactivity of organometallic compounds

Course Outline:

UNIT-I: Inorganic Photo Chemistry and Photo Electron Spectroscopy

Unimolecular charge-transfer photochemistry of cobalt (III) complexes – mechanism of CTTM, photoreduction – ligand-field photochemistry of chromium (III) complexes – Adamson's rules, photoactive excited states, V-C model – photophysics and photochemistry of ruthenium – polypyridine complexes, emission and redox properties. Photoelectron Spectroscopy

PES - Theory, Types, origin of fine structures - shapes of vibrational fine structures – adiabatic and vertical transitions, PES of homonuclear diatomic molecules (N_2, O_2) and heteronuclear diatomic molecules (CO, HCl) and polyatomic molecules (H_2O, CO_2, CH_4, NH_3) – evaluation of vibrational constants of the above molecules, Koopman's theorem- applications and limitations.

UNIT-II: Nuclear and Radiation Chemistry 9Hrs

Properties of nucleus – different types of nuclear forces , Nuclear structure and nuclear stability, Nuclear models- – liquid drop model, shell model of nucleus, Radioactivity and nuclear reactions, nuclear reactions induced by charged particles – Q value – nuclear reaction cross section, significance and determination – theory of nuclear fission, nuclear fusion, stellar energy. Hot atom chemistry, Nuclear fission and fusion reactors. The interaction of nuclear radiations with matter. Radiation hazards and therapeutics. Detectors and their principles. Tracer Application of

radioisotopes in agriculture, industry and medicine. Isotope dilution and radio-activation methods of analysis.

UNIT-III: Applications of IR, Raman and NMR Spectroscopy 9Hrs

IR spectroscopy- Introduction, selection rules, stretching frequency of some inorganic ions- effect of coordination on the stretching frequency- sulphato, carbonato, sulphito, aqua, nitro, thiocyanato, cyano, thiourea, DMSO complexes.

Raman spectroscopy – Introduction, combined applications of IR and Raman spectroscopy in the structural elucidation of N_2O, ClF_3, NO_3-, ClO_4, metal carbonyls.

NMR spectroscopy- Introduction, structural assessment of simple inorganic compounds, applications of 1H, 15N,19F, 31P-NMR spectroscopy in structural problems, fluxional molecules, quadrupolar nuclei- effect in NMR spectroscopy, shift reagents- applications.

UNIT-IV: ESR and Mössbauer Spectroscopy 9Hrs

ESR spectroscopy-Introduction, presentation of esr spectra g and A parameters, spin densities, Mc-Connel relationship, factors affecting the magnitude of g and A. Zero field splitting, Kramer's degeneracy, esr spectra of V(II), Mn(II) Fe (II), Co (II), Ni(II), Cu (II) complexes, bis(salicylaldimine)copper (II), $[(NH_3)_5Co\text{-}O_2\text{-}Co(NH_3)_5]^{5+}$.

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

UNIT-V: Organometallic Chemistry 9Hrs

Types of organometallic compounds on the basis of the nature of M-C bond. EAN rule: 18e- and 16e- rules – determinator of oxidation state, configuration, coordination number of the metal centre – Types and application 18e- / 16e- rules. Carbonyls – isolated concept.- Structure of carbonlys (simple and polynuclear) Nitrosyls – bridging and terminal nitrosyls, bent and linear nitorsyls. Dinitrogen compounds donors – Alkyl and Aryl – preparation and properties; chain carbon donors – olefins, acetylene and allyl complexes – synthesis, structure and bonding; cyclic carbon donors – (metallocene) – synthesis, structure and bonding.

Important types of reactions of organometallic compounds – substitution – electrophilic and nucleophilic attack on ligands; carbonylation and decarbonylation; oxidative addition and reductive elimination, insertion and deinsertion (elimination). Template synthesis of macrocyclic ligands.

Mapping of Cos to POs and PSOs

CO	Correlation level																Cogniti ve level
	PO									PSO							
	1	2	3	4	5	6	7	8	1	2	3	4	5	6	7	8	
CO1	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K1
CO2	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K2
CO3	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K3
CO4	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K4
CO5	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5
CO6	L	L	L	L	H	L	L	L	L	L	L	L	H	L	L	L	K5,K6

References

1. E. A. V. Ebsworth, Structural Methods in Inorganic Chemistry, 3rd Ed ELBS, Great Britain, 1987.
2. H. J. Arniker, Essentials of Nuclear Chemistry, 2nd Ed, Wiley Eastern Co, 1987.
3. G. Friedlander, J. W. Kennedy and J. M. Miller, Nuclear and Radiochemistry, Wiley, 1964.
4. H. Kaur – "Spectroscopy", 3rd Ed., Pragati Prakasan Publications, Meerut, 2006.
5. R. S. Drago, Physical methods in inorganic chemistry; Affiliated East-West Press Pvt. Ltd., New Delhi, 2012.
6. R. S. Drago, Physical methods in chemistry; Saunders college publications, Philadelphia, 1992.
7. P. J. Wheatley, The determination of molecular structure, 2nd edition, Dover Publications, Mineola, 1981.
8. C. N. Banwell, Fundamentals of molecular spectroscopy 4th edition, McGraw Hill Education, Noida, 1994.

Supportive Course (Mandatory): ENVIRONMENTAL CHEMISTRY (E-Pathshala)

L	T	P	C
4	-	-	3

Course Code:

Course Objectives:

1. To educate the students on atmosphere, water quality analysis and various pollutions
2. To impart understanding on Environmental issues

Course Prerequisites:

The pre-requisite for studying the course on Environmental Chemistry is basic knowledge on the atmosphere, pollution types and sources

Course Outcomes (Cos):

At the end of the course the students should able to

CO1: Learn about the air, land, and water pollutions.

CO2: gain knowledge of various environmental segments, their interaction among each other and how they are contaminated due to man-made activities on the earth.

CO3: Aware about environment and educate others that how our planet is getting spoiled and what are the remedies to stop this pollution.

CO4: Explain the collection, processing, advanced treatment and reuse of waste water

Course outline:

Unit I **9Hrs**

Atmosphere: Introduction – structure and evolution of the atmosphere – heat budget – Biogeochemical cycle of carbon, nitrogen, sulphur, phosphorous, and oxygen – Hydrosphere: Chemical Composition of water bodies, Composition of specific water body, properties of water and hydrological cycle

Unit II **9Hrs**

Water pollution: Introduction – classification of water pollutants – Water Quality Parameters - Water Quality Criteria for Classification of Water Bodies – Waterborne diseases – analytical techniques for measuring water quality parameters – Wastewater purification – advanced wastewater treatment

Unit III **9Hrs**

Soil pollution – soil characters, composition, soil organisms, soil profile, soil reactions, micro and macro nutrients – soil pollution – sources (fertilizers and pesticides) and effects – plastic pollution: sources, impact on environment, effects, prevention and control – waste treatment – heavy metal pollution: sources, toxicity, prevention and control

Unit IV **9Hrs**

Air pollution: composition of atmosphere – particles, ions and radicals with reactions - Chemical and photochemical reaction in the atmosphere, Smog - Oxides of Nitrogen, Sulphur, Carbon and Their Effects - Pollution by chemicals, petroleum, minerals and chlorofluorohydrocarbons – green house effects – air pollution controls and continuous monitoring – analytical methods of measurements of air pollutants

Unit V **9Hrs**

Industrial water pollution: pulp, paper industry and agrochemicals - Cement industry, Sugar industry, Distillery, Paper and Pulp industries – thermal power plant – Nuclear Power plant – Environmental Issues of Metallurgy – Radionuclides analysis and Waste Management – Environmental issues of polymer and drug industry – Biodegradability and Decomposition – Bhopal Gas Tragedy – Environmental Friendly practices and industrial pollution.

Mapping of Cos to POs and PSOs

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CO2	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K2
CO3	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K3
CO4	L	L	L	L	H	H	L	L	L	L	L	L	H	H	L	L	K4

References

1. Dara SS (2000) A text book of Environmental chemistry and pollution control, S. Chand Company, New Delhi
2. Sharma BK, Kaur H (2000) Environmental Chemistry, Goel Publishing House, Meerut, India
3. APHA 1975, Standard methods for the examination of wastewater, AWWA, New york
4. Manahan, Stanley E. Fundamentals of Environmental Chemistry Boca Raton: CRC Press LLC,2001
5. Sonja Krause, Herbert M. Clark, James P. Ferris, Robert L. Strong Chemistry of the Environment, Elsevier Science &Technology Books 2002
6. Eugene R. Weiner Applications of Environmental Chemistry 2000 CRC Press, LLC
7. By Clair N.Sawyer, Perry L. McCarty, Gene F.Parkin Chemistry for environmental engineering and science (5th edition) McGrawHill Professional

Core – 12: APPLICATIONS OF NANOTECHNOLOGY

L	T	P	C
4	-	-	4

Course Code:

Course Objectives:

1. Understand the most prominent Nano devices and applications
2. To study the applications and characters of quantum materials, nanosensors, and solar cells
3. To study the applications of nanomaterials in medicinal and pharmaceutical field

Course Pre-requisites:

Acquiring detailed knowledge in nanomaterials and their applications in various field

Course outcome (COs)

At the end of the course the students should able to

CO1:Define and explain the magnetic properties of nano ceramics

CO2:Study the sensor characterization and modes of packaging

CO3:Apply the sensing of physical parameters sensed to fabricate appropriate sensors. Understand the lithography and sensor use of nanomaterials

CO4:Realize how nanotechnology can be tailored and used for biomedical purposes, catalyst, nanorobotics, engineering.

CO5: Elucidate food quality, safety and security of agricultural product, packaging and distribution, nanomaterials for food applications.

CO6: Students will be able to familiar in the medicinal applications of nanomaterials especially about targeted drug delivery

Course Outline

Unit I **9Hrs**

Nano ceramics: Dielectrics, ferroelectrics and magnetoceramics, Magnetism; Dia-, Para-, Ferro-, Antiferro-, Ferri-magnetism, Magnetic properties; Gaint magnetoresistance, Tunneling magnetoresistance, Colossal magnetoresistance, Superparamagnetism High Tc materials: YBCO and Bi-systems (Brief idea), Superconducting nano-materials & their properties and applications.

Unit-II **9Hrs**

Nanosensors: Temperature Sensors, Smoke Sensors, Sensors for aerospace and defense: Accelerometer, Pressure Sensor, Night Vision System, Nano tweezers, nano-cutting tools, Integration of sensor with actuators and electronic circuitry Biosensors. Nanotechnology Enabled

Sensors - Static and Dynamic Characteristics; - Gas Sensing with Nanostructured Thin Films, Nano-sensors based on Nucleotides and DNA.

Unit-III **9Hrs**

Nanoelectronics: Microelectronics- molecular electronics- photonics–photolithography–carbon nanotubes (CNT) in electronic applications- State of Art Ion-beam exchange in Nanostructure material. Nanostructure based Photovoltaic Cells. Solar Cells - Band Diagram and Operational Principle of Nanocrystalline Solar Cells - Quantum Dot Sensitizer

Unit IV **9Hrs**

Biomedical applications: Nanomedicine and Nanopharmaceutical: Principles of nanomedicine – impact of nanotechnology in medicine- nanoparticles delivery for cancer therapy – Bioactive nanomaterials in medicine- Nanodiagnostics - Nanoarrays for diagnostics-nanoparticles for molecular diagnostics nanoarrays- protein nanobiochip - Nanobiosensor-CNT biosensor-DNA biosensor. QD Bionanostructures - Characterization of QD Biostructures – Drug delivery – ADME hypothesis - Targeted Nano particles for drug delivery-Polymers nanotubes - lipid nanoparticles - vaccination - cell therapy -Gene therapy

Unit V (Nanostructured Food and Packaging Materials) **9Hrs**

Natural Food Nanostructures - Naturally Occurring Food Nano substances and Nanostructures - Designing Food Nanostructures - The Status of Natural Nanostructures in Food - Nanomaterials for (Health)food Applications - Nano-sized Food Ingredients and Additives in Relation to Digestion of Food - Nanotechnologies in Food Packaging - Improvement of Mechanical Properties through Nanocomposites - Improvement of Barrier Properties - Improvement of the Performance of Bio-based Polymers - Surface Biocides - Active Packaging Materials - Intelligent Packaging Concepts.

Mapping of Cos to POs and PSOs

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	PO									PSO							
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CO2	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K2
CO3	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K3

CO4	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K4
CO5	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K5
CO6	L	L	L	L	H	M	L	L	L	L	L	L	H	M	L	L	K6

References

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2.Patenting Nanomedicines: Legal Aspects, Intellectual Property and Grant ..., edited by Eliana B. Souto

3.NanoBioTechnology: BioInspired Devices and Materials of the Future, By Oded Shoseyov, Ilan Levy

4.Handbook of Clinical Nanomedicine: Nanoparticles, Imaging, Therapy, and ..., edited by Raj Bawa, Gerald F. Audette, Israel Rubinstein

5.Nanotechnology-Enabled Sensors, By Kourosh Kalantar-zadeh, Benjamin Fry

6.Nanomedicine and Drug Delivery, edited by Mathew Sebastian, Neethu Ninan, A. K. Haghi

7.Nanopharmaceutics: The Potential Application of Nanomaterials, By Xing-Jie Liang

8.Biological and Pharmaceutical Applications of Nanomaterials, edited by Polina Prokopovich

9.K. Goser, et al, "Nanoelectronics and Nanosystems", Springer, 2004.

10. Biointeractions of Nanomaterials, edited by Vijaykumar B. Sutariya, Yashwant Pathak

11. Environmental Applications of Nanomaterials: Synthesis, Sorbents and Sensors, By Glen E. Fryxell, Guozhong Cao

12. Pharmaceutical Nanotechnology: Fundamentals and Practical Applications, By Costas Demetzos

13. The Handbook of Nanomedicine, By Kewal K. Jain

14. CRC Handbook of Thermoelectrics, Ed. CR Rowe

Industrial Internship

Project and Viva-Voce