COURSES OF STUDIES

FOR POST GRADUATE DEGREE IN CHEMISTRY
(SEMESTER SYSTEM)

Session: 2023-24

DEPARTMENT OF CHEMISTRY
INDIRA GANDHI NATIONAL TRIBAL UNIVERSITUY
AMARKANTAK, MADHYA PRADESH-484887

VISION

To build the Department of Chemistry into a Centre of academic excellence with total commitment to ensure quality education in Chemistry and allied fields, with a holistic approach towards a better life, environment and society.

MISSION

M1: Promotes fundamentals of Chemistry through UG and PG courses

M2: Offer high end-research projects on concept-theory-practical topics.

M3: To provide excellent teachers, entrepreneurs and innovative independent researchers.

M4: Become a nationally recognized center for chemical sciences and to establish state of Art centralize research facility.

VALUES

- **Collaboration**
- **Creativity**
- **Diverse perspective**
- **Empowerment**
- **Informed practices**
- **Professionalism**

PROGRAM OUTCOMES

[PO.1]. Critical Thinking: Take informed actions after identifying the assumptions that frame our thinking and actions, checking out the degree to which these assumptions are accurate and valid, and looking at our ideas and decisions (intellectual, organizational, and personal) from different perspectives.

[PO.2]. Self-directed and Life-long Learning: Acquire the ability to engage in independent and life-long learning in the broadest context socio-technological changes.

[PO.3]. Social Interaction: Elicit views of others, mediate disagreements and help reach conclusions in group settings.

[PO.4]. Effective Citizenship: Demonstrate empathetic social concern and equity centered national development, and the ability to act with an informed awareness of issues and participate in civic life through volunteering.

[PO.5]. Ethics: Recognize different value systems including your own, understand the moral dimensions of your decisions, and accept responsibility for them.

[PO.6]. Environment and Sustainability: Understand the issues of environmental contexts and sustainable development.

[PO.7]. Effective Communication: Speak, read, write and listen clearly in person and through electronic media in English and in one Indian language, and make meaning of the world by connecting people, ideas, books, media and technology.

PROGRAM SPECIFIC OUTCOMES

[PSO.1]. Develop knowledge, understanding and expertise in their chosen field of chemical science.

[PSO.2]. Develop an understanding of eco-friendly chemical processes and impact of chemistry on health and environment.

[PSO.3]. Understand theoretical concepts of instruments that are commonly used in most chemistry fields as well as interpret and use data generated in instrumental chemical analyses.

[PSO.4]. Provide opportunities to excel in academics, research or Industry

P.G. PROGRAM ARTICULATION MATRIX

SEMESTER	COURCE CODE	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PSO1	PSO2	PSO3	PSO4
I	CHM T 411	2	2	2	1	0	1	2	2	1	0	2
	CHM T 412	2	2	2	1	0	1	2	2	1	0	2
	CHM T 413	2	2	0	1	0	1	1	2	1	2	2
	CHM P 411	3	2	2	1	1	2	0	3	2	0	3
	CHM P 412	3	0	1	3	1	3	3	3	3	3	3
II	CHM T 421	3	2	1	2	1	3	2	3	2	3	3
	CHM T 422	3	2	3	1	1	2	2	3	1	0	2
	CHM T 423	3	2	0	3	0	2	1	3	3	3	3
	CHM T 604	3	2	0	1	0	2	3	3	2	0	3
	CHM P 421	3	0	2	2	2	0	0	1	3	3	1
	CHM P 422	2	2	0	1	2	1	2	2	0	0	2
III	CHM T 511	3	2	1	3	1	2	3	3	0	2	3
	CHM T 512	3	2	2	1	2	3	3	3	0	0	3
	CHM T 513	2	2	0	1	0	1	2	2	1	2	2
	CHM T 606	3	2	0	0	0	2	3	3	2	0	3
	CHM P 511	3	0	2	1	2	2	3	3	2	3	3
	CHM P 512	2	1	1	3	2	1	3	3	2	0	3
IV	CHM T 521	3	2	1	1	1	2	3	1	1	0	3
	CHM T 608	3	2	2	3	2	2	3	2	2	0	3
	CHM P 522	3	2	0	0	0	2	2	1	0	0	3
AVERAGE		2.7	1.65	1.1	1.5	0.9	1.75	2.15	2.4	1.45	1.05	2.6

POST GRADUATE PROGRAMME STRUCTURE DEPARTMENT OF CHEMISTRY

Post graduate program comprising two years, will be divided into 4 (four) semesters each of six months duration.

Year	Semesters	
First Year	Semester I	Semester II
Second Year	Semester III	Semester IV

PART –I, First Semester

PAPER NO/CODE	NAME OF THE COURSE	MARKS		TOTAL MARKS	DURATION (HRS) OF EXAM (END TERM)	CREDIT HOURS
		END TERM	MID TERM			
CHM T 411 (THEORY)	PHYSICAL CHEMISTRY- I	60	40	100	3	4
CHM T 412 (THEORY)	INORGANIC CHEMISTRY- I	60	40	100	3	4
CHM T 413 (THEORY)	ORGANIC CHEMISTRY- I	60	40	100	3	4
CHM P 411 (PRACTICAL)	ORGANIC PRACTICAL-I	-	-	50	3	2
CHM P 412 (PRACTICAL)	INORGANIC PRACTICAL-I	-	-	50	3	2
Total				400		16

PART –II, Second Semester

PAPER NO	NAME OF THE COURSE	MARKS		TOTAL MARKS	DURATION (HRS) OF EXAM (END TERM)	CREDIT HOURS
		END TERM	MID TERM			
CHM T 421 (THEORY)	PHYSICAL CHEMISTRY -II	60	40	100	3	4
CHM T 422 (THEORY)	INORGANIC CHEMISTRY- II	60	40	100	3	4
CHM T 423 (THEORY)	ORGANIC CHEMISTRY- II	60	40	100	3	4
CHM T 604 (THEORY)	INSRUMENTAL METHODS OF ANALYSIS (ANALYTICAL CHEMISTRY)	60	40	100	3	4
CHM P 421 (PRACTICAL)	PHYSICAL PRACTICAL-I	-	-	50	3	2
CHM P 422 (PRACTICAL)	ORGANIC PRACTICAL-II	-	-	50	3	2
Total				500		20

PART –III, Third Semester

PAPER NO	NAME OF THE COURSE	MARKS		TOTAL MARKS	DURATION (HRS) OF EXAM (END TERM)	CREDIT HOURS
		END TERM	MID TERM			
CHM T 511 (THEORY)	PHYSICAL CHEMISTRY- III	60	40	100	3	4
CHM T 512 (THEORY)	INORGANIC CHEMISTRY- III	60	40	100	3	4
CHM T 513 (THEORY)	ORGANIC CHEMISTRY- III	60	40	100	3	4
CHM T 606 (THEORY)	INTRODUCTION TO NANOMATERIAL AND NANOTECHNOLOGY	60	40	100	3	4
CHM P 511 (PRACTICAL)	PHYSICAL PRACTICAL-II	-	-	50	3	2
CHM P 512 (PRACTICAL)	INORGANIC PRACTICAL-II	-	-	50	3	2
Total				500		20

PART –IV, Fourth Semester

PAPER NO	NAME OF THE COURSE	MARKS		TOTAL MARKS	DURATION (HRS) OF EXAM (END TERM)	CREDIT HOURS
		END TERM	MID TERM			
CHM T 521 (THEORY)	MOLECULAR SPECTRISCOPY	60	40	100	3	4
CHM T 608 (THEORY)	ORGANIC CHEMISTRY -IV	60	40	100	3	4
CHM P 522 (THEORY)	PROJECT DISSERTATION	--	--	200	3	12
Total				400		20
20 PAPERS	Grand Total	1800				76

*Pass percentage

1. The minimum marks required to pass any paper shall be 40 percent and 40 percent in aggregate of a semester.

2. No students will be allowed to avail more than three chances to pass in any paper inclusive of first attempt.

FIRST SEMESTER

PAPER CODE: CHM T 411: PHYSICAL CHEMISTRY –I

(Thermodynamics, Catalysis, and Electro- & Surface Chemistry)

Full Mark 100 (60 + 40)

Course Objectives: The learners should be able to apply, analyze and evaluate the kinetics of catalysis, thermodynamics, and electro chemistry of solutions, over potential and corrosion & surface active agents and surface chemistry.

A. **Course Outcomes:** At the end of the course, students will be able to

[CHM T 411.1]. Recall basic concepts of thermodynamics, excess function for non-ideal solutions.
[CHM T 411.2]. Understand the heterogeneous catalysis via surface reactions.
[CHM T 411.3]. Understand the Kinetics of homogeneous catalysis.
[CHM T 411.4]. Discuss the electrical double layer and metal/electrolyte interface.
[CHM T 411.5]. Discuss the basics concepts of surface tension and surface active agents.

B. **Unit – I: Thermodynamics**

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential, and entropies. Thermodynamics of open systems: partial molal properties, partial molal free energy, partial molal volume and partial molal heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity. Non-ideal system: excess function for non-ideal solutions. Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solution; determination of activity and activity coefficients; ionic strength.

Unit – II: Heterogeneous Catalysis

***Heterogeneous Catalysis* (*Surface Reactions*):** Kinetics of uni-molecular reactions- inhibition and activation energy. Bimolecular surface reactions - reactions between a gas molecule and an adsorbed molecule, reaction between two adsorbed molecules. Effect of temperature on surface reaction promoters and poisons.

Unit – III: Homogeneous Catalysis

Kinetics Homogeneous Catalysis: Nature of surface, concept of active centers. Kinetics of enzymatic reactions: Michaelis-Menten equation, Lineweaver-Burk and Eadie Analyses, enzyme inhibition (competitive, non-competitive and uncompetitive inhibition), effect of temperature and pH of enzymatic reaction; acid – base catalysis and their mechanism.

Unit – IV: Electrochemistry

***Electrochemistry of Solution*:** Debye-Hückel treatment and its extension, ion solvent interaction. Debye-Hückel-Jerum mode. Thermodynamics of electrified interface equation. Derivations of electrocapillary, Lippmann equation (surface excess); method of determination structure of electrified interfaces. Gouy-Chapmann, Stern, Graham-Devanathan Mottwatts, Tobin, Bockris, Devanathan Models.

Over Potential: Exchange current density, derivation of Butler-Volmer equation, Tofel plot. Quantum aspect of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling.

Corrosion: Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention method.

Unit – V: Surface Chemistry

***Surface Tension*:** Capillary action, pressure difference across curved surface (Laplace equation), vapor pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film and liquids (electro-kinetic phenomenon), catalytic activities at surface.

***Surface Active Agents*:** Classification of surface-active agents. Micellization, hydrophobic interaction, critical micellar concentration (CMC), factor affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro-emulsion reverse micelles.

C. REFERENCE BOOKS:

1. P. Atkins, J. d. Paula and K. James, *Physical Chemistry*, 11th Ed., Oxford University Press, **2018**.
2. J. Bockris, O'M and A. K. N. Reddy, *Modern Electrochemistry: Ionics, Vol. 1*, 2nd Ed., Springer, **2006**.
3. J. Bockris, O'M, A. K. N. Reddy and M. Gamboa-Aldeco, *Modern Electrochemistry: Findamentals of Electrodics, Vol. 2A*, 2nd Ed., Springer, **2006**.
4. D. R. Crow, *Principles and Applications of Electrochemistry*, 4th Ed., Blackie Academic & Professional, **1994**.
5. S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press P. Ltd, **2003**.
6. K. L. Kapoor, *A Text Book of Physical Chemistry: Dynamics of Chemical Reactions, Statistical Theromodynamics, Macromolecules and Irreversible Processes, Vol. 5*, 5th Ed., McGraw-Hill, **2015**.
7. K. J. Laidler, *Chemical Kinetics*, 3rd Ed., Pearson, **2011**.
8. R. G. Mortimer, *Physical Chemistry*, 3rd Ed., Academic Press, **2008**.
9. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Ed., Vishal Publishing Co., **2018**.
10. J. Rajaram and J. C. Kuriacose, *Kinetics and Mechanisms of Chemical Transformations*, Penguin Books Ltd, **2009**.
11. R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, 2nd Ed., Oxford University Press, **2007**.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSE	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 411.1	Recall basic concepts of thermodynamics, excess function for non-ideal solutions.	3		2				2	2			2
CHM T 411.2	Understand the heterogeneous catalysis via surface reactions.	2	2				2		2	1		1
CHM T 411.3	Understand the Kinetics of homogeneous catalysis.	1			2		2				3	2
CHM T 411.4	Discuss the electrical double layer and metal/electrolyte interface.	2		1			2			2	2	2
CHM T 411.5	Discuss the basics concepts of surface tension and surface active agents.	2		1		3		2	2			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 412: INORGANIC CHEMISTRY –I

(Transition and Inner Transition Metal Chemistry)

Full Mark 100 (60 + 40)

Course Objectives: To learn the Co-ordination chemistry, electronic spectra, magnetic properties of transition metal compounds. Understand the mechanism of electron transfer reactions and involvement of reactive species and understand their structure and reactivity. Coordination chemistry, spectral and magnetic properties and usages of d-series compounds

A. **Course Outcomes:** At the end of the course, students will be able to

[CHM T 412.1]. Understand the Co-ordination chemistry of transition metal compounds.
[CHM T 412.2]. Learn about the electronic spectra of transition metal complexes and their studies.
[CHM T 412.3]. Learn about the magnetic properties of transition series metals, lanthanides and actinides.
[CHM T 412.4]. Apply concepts on Inorganic reaction mechanism and electron transfer reactions.
[CHM T 412.5]. Understand the spectral and magnetic properties and usages of d-series compounds.

B. **SYLLABUS**

Unit – I: Co-ordination Chemistry

Experimental evidence of metal-ligand overlap, spin orbit coupling constant and interelectronic coupling parameters in complex ion terms-vs-free ion terms, Nephelauxetic effect, *d*-orbital splitting in octahedral, Jahn-Teller distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes, CFSE for d^1 to d^{10} systems, pairing energy, low-spin and high-spin complexes and magnetic properties, Crystal field activation energy, hole formalism, Tetrahedral distortion and Jahn Teller effect, Static and Dynamic Jahn-Teller effect, Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stabilization of complexes (Irving Williams order). Colour and spectra, Kinetic aspects of crystal field stabilization. Adjusted CFT, Limitations of CFT, Labile and inert complexes.

Unit – II: Electronic Spectra of Transition Metal Complexes

Microstates, Russell-sander's terms, determination of ground and excited state terms of d^n ions; Orgel diagrams (qualitative approach) and Tanabe-Sugano diagram, selection rules for spectral transitions, *d-d* spectra of d^n ions and crystal field parameters, Nephelauxetic series, Electronic Spectra UV-Vis, charge transfer, colors, intensities and origin of spectra. MOT to rationalize σ and π interactions in octahedral, square planar and tetrahedral metal complexes. Symmetry designations of LGOs and MOs. Simplified MO diagrams.

Unit – III: Magneto Chemistry

Basic principles of magnetism, Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, determination of magnetic susceptibility, application of Van Vleck susceptibility equation, Magnetic properties and coordination compounds Spin and orbital moments, spin – orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable temperature magnetic moments and spin crossover. Magnetic properties of first transition series metal ions, lanthanides and actinides, Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples). Magnetic exchange interactions. ESR spectroscopy, Basic concept of Single Molecule Magnets (SMM), properties, examples and application of SMMs.

Unit – IV: Inorganic Reaction Mechanism

Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ($\Delta S^{\#}$, $\Delta H^{\#}$, $\Delta V^{\#}$), mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-condon principle (non mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalyzed substitution reactions.

Unit - V: Chemistry of Elements

d-Series Elements: Electronic configuration, oxidation states; aqueous, redox and coordination chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d, 4d, and 5d elements with references to Ti-Zr- Hf , V-Nb-Ta, Cr- Mo- W, Mn-Tc-Re and Pt group metals. Occurrence and isolation in respect of V, Mo, W, Re, Pt. Iso- and heteropolyoxometalates with respect to V, Mo, and W: synthesis, reactions, structures, uses, metal-metal bonded dinuclear d-metal complexes (examples), bonding in dirhenium complexes.

C. Reference Books:

1. J. D. Lee: *A new Concise Inorganic Chemistry*, EL.B.S.
2. D. F. ShriverandP. W.Atkins: *Inorganic Chemistry*, Oxford UniversityPress.
3. Douglas, McDaniel and Alexander: *Concepts and Models in Inorganic Chemistry*, John Wiley.
4. B. R. Puri, L. R. Sharma, and K. C. Kalia: *Principle of Inorganic Chemistry*, Milestone Publisher, New Delhi 2010.
5. W. U. Malik, G. D. Tuli, and R. D. Madan: *Selected Topic in Inorganic Chemistry*, S. Chand & Company Ltd, New Delhi, 1998.
6. J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4th Pearson, New Delhi, 2006.
7. F. A Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann: *Advanced Inorganic Chemistry*, Eds: 6th, Wiley-India, New Delhi, 2010.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 412.1	Understand the Co-ordination chemistry of transition metal compounds	2					1	2		1		2
CHM T 412.2	Learn about the electronic spectra of transition metal complexes and their studies.	2		3			1	2	2	1		2
CHM T 412.3	Learn about the magnetic properties of transition series metals, lanthanides and actinides.	2	2	2	3	1			2			1
CHM T 412.4	Apply concepts on Inorganic reaction mechanism and electron transfer reactions.	1	1						2			3
CHM T 412.5	Understand the spectral and magnetic properties and usages of d-series compounds.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 413: ORGANIC CHEMISTRY –I

(Organic Reaction Mechanism and Stereochemistry)

Full Mark 100 (60 + 40)

Course Objectives: To learn the involvement of reactive intermediates and understand their structure and reactivity in aliphatic and aromatic compounds through various organic reactions.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 413.1]. Understand the physical properties (thermodynamic and kinetic) of organic reactions.
[CHM T 413.2]. Learn about substitution, addition, and elimination of organic reactions.
[CHM T 413.3]. Understand the symmetry properties, stereoisomerism and stereospecific reactions.
[CHM T 414.4]. Learn the principle and concepts of organic compounds chirality and conformations.
[CHM T 415.5]. Understand the concepts of conformation and stereo selective reactivity.

B. **SYLLABUS**

Unit – I : Physical Organic Chemistry

Thermodynamic and kinetic requirements of a reaction: Transition state theory, Hammond's postulate, Kinetic vs Thermodynamic control
Acids and Bases
Determining the mechanism of a reaction: Detection and trapping of intermediates, Cross-over experiments, kinetic isotopic effect-primary kinetic and secondary kinetic isotopic effect

Unit – II: Substitution, Addition, and Elimination Reactions

Substitution Reaction: Aliphatic nucleophilic substitution- SN1, SN2, SNi mechanism, classical and nonclassical carbocations, phenonium ions, NGP-in substation reactions. Effect of solvent, structure, nucleophile and leaving group on rate of SN1, and SN2 reaction. Electrophilic aromatic substitution and Nucleophilic aromatic substitutions. Mechanism and stereo chemical aspects of substitution reactions.
Addition Reaction: Addition to carbon-carbon multiple bonds, addition to carbon-heteroatom multiple bonds, electrophilic, nucleophilic and free radical addition reactions. Mechanism and stereo chemical aspects of addition reactions.
Elimination Reaction: E1, E2, E1cb mechanisms, orientation and stereochemistry in elimination reaction, reactivity effect of structure, attacking and leaving group, competition between elimination and substitution, syn-eliminations.

Unit – III: Symmetry Operation and Stereoisomerism

Simple or proper axis of symmetry, plane of symmetry, centre of symmetry and improper or rotation-reflection of symmetry. Enantiomerism and diastereomerism, conventions for configurations D-L and R-S systems, Threo and erythro nomenclature. Measurement of optical purity, enantiomeric excess. Stereoselective and Stereospecific reactions. Molecules with tri- and tetra coordinated chiral centres. Molecules with two or more chiral centres.

Unit – IV: Chirality and Conformations

Axial and Planar Chirality: Principles of axial and planar chirality. Stereochemistry of allenes, Stereochemistry of biphenyl derivatives and atropisomers. Stereochemistry of spiranes, Stereochemistry of molecules with planar chirality, Helicity.
Conformations & Stereoisomerism of Acyclic and Cyclic Systems: Molecular mechanics and conformations, Conformations of a few acyclic molecules, Conformations of cyclic systems: monocyclic compounds (mono, di- and poly substituted cyclohexanes); Conformations of fused ring and bridged ring compounds.

Unit – V: Dynamic Stereochemistry

Conformation and Reactivity: Conformation, reactivity and mechanism: Cyclic systems (Nucleophilic substitution reaction at ring carbon, Addition reaction to double bonds, Elimination reactions, NGP reactions). Conformation, reactivity and mechanism: Acyclic systems (addition, Elimination and NGP participation). Formation and reaction of enols and enolates. Reduction of cyclohexanes with hydride reagents.

Stereoselective Reactions: Principle of stereoselectivity, asymmetric synthesis and asymmetric induction, Acyclic stereoselections (addition of nucleophiles to carbonyl compounds, aldol reactions, addition to allyl metal and allyl boron compound to carbonyl compounds), Diastereoselections in cyclic systems (Nucleophilic addition to cyclic ketones, alkylations, catalytic hydrogenations).

C. References:

1. Stereochemistry of organic compound: Principle and Applications –By D. Nasipuri
2. Organic Chemistry, Oxford-By J. Clayden, N. Greeves, S. Warren and P. Wothers
3. Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, Sixth Edition-By Michael B. Smith, Jerry March
4. Advance Organic Chemistry (part A)-By A. Carey and R.J. Sundberg
5. Stereochemistry of carbon compounds-By E.L. Eliel
6. Guide book to Reaction Mechanism-By Peter Sykes

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 413.1	Understand the physical properties (thermodynamic and kinetic) of organic reactions.	2					1	2		1		2
CHM T 413.2	Learn about substitution, addition, and elimination of organic reactions.	2		3			1	2	2	1		2
CHM T 413.3	Understand the symmetry properties, stereoisomerism and stereospecific reactions.	2	2	2	3	1			2			1
CHM T 413.4	Learn the principle and concepts of organic compounds chirality and conformations.	1	1						2			3
CHM T 413.5	Understand the concepts of conformation and stereo selective reactivity.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM P 411: INORGANIC CHEMISTRY PRACTICAL - I

Full Mark 50

Course Objectives: The learners should be able to apply the principles of semi-micro qualitative analysis and analytical techniques in inorganic chemistry for compound identification of the metal ion and separation of sugars, amino acids by using the chromatographic separation techniques (paper, T.L.C. and Ion exchange).

A. Course Outcomes: At the end of the course, students will be able to

- Understand the Semi-micro qualitative analysis of unknown mixture containing eight radicals.
- Learn about the Chromatographic separation techniques and identify the metal ion components and separation of sugars, amino acids.
- Calculation of standard deviation from the results obtained by redox and complexometry titrations

B. SYLLABUS

A. Qualitative Analysis Semi-micro qualitative analysis of mixture containing eight radicals including two less common metal from among the following:

(1) *Basic Radicals*: Ag^{+}, Pb^{2+}, Bi^{3+}, Cu^{2+}, Cd^{2+}, As^{3+}, Sb^{3+}, Sn^{4+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}, Ce^{3+}, Th^{4+}, Zr^{4+}, W^{6+}, Te^{4+}, Ti^{4+}, Mo^{6+}, V^{5+}, Be^{2+}.

(2) *Acid Radicals* : Carbonate, Sulphite, Sulphide, Nitrite, Nitrate, Acetate, Fluoride. Chloride, Bromide, Iodide, Sulphate, Borate, Oxalate, Phosphate, Silicate, Thiosulphate, Ferrocyanide, Ferricyanide, Thiocyanide, Chromate, Arsenate and Permanganate.

B. Chromatographic Separation

Use paper chromatography to separate and identify the metal ion components of an unknown solution. Chromatographic separation of sugars, amino acids by paper, T.L.C. and Ion exchange.

C. Standard Deviation

Calculation of standard deviation from the results obtained by redox titration of Fe(III) against standard solution of $K_2Cr_2O_7$.

Calculation of standard deviation from the results obtained by complexometry method of hardness (Ca^{2+}) of water using EDTA.

Reference Books:

1. A.I. Vogel: *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
2. A.I. Vogel: *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.
3. B.D. Khosla: *Senior Practical Physical Chemistry*, R. Chand & Co.
4. P. C. Comboj: *University Practical Chemistry*, Vishal Publishing Co. Jalandhar.

PAPER CODE: CHM P 412: ORGANIC CHEMISTRY PRACTICAL - I

Full Mark 50

Course Objectives: The learners should be able to: Apply principles of Separation and Purification techniques in organic reactions. Analyze the organic binary mixtures and synthesis of organic compounds.

A. SYLLABUS

Part A: Techniques of Separation and Purification

- Fractional Distillation of a mixture of liquids
- Distillation under reduced pressure
- Chromatographic separation (Paper chromatography and Thin Layer Chromatography)

Part B: Analysis of Organic Binary Mixture

Separation and Identification of organic compounds from the given binary mixtures. (Complete study of determination of organic compound with melting point and preparation of a suitable derivative)

Part C: Preparation of Organic Compounds (Single Stage Preparation)

Representative reactions to be covered:

- Electrophilic aromatic substitution reaction (Friedel-Crafts Reaction, halogenation, nitartion and sulphonation reaction)
- Acetylation reaction
- Diels-Alder reaction
- Condensation reaction
- Cannizzaro reaction
- Oxidation reaction
- Reduction reaction
- Rearrangement reaction
- Esterification
- Diazotization reaction
- Sandmeyer reaction

B. Reference Books:

1. A. I. Vogel: *Practical Organic Chemistry*
2. F. G. Mann and B. C. Saunders: *Practical Organic Chemistry*
3. J. Leonard, B. Lygo and G. Proctor: *Advanced Practical Organic Chemistry*.
4. Addison Ault: *Techniques and Experiments for Organic Chemistry*, University Science Book
5. R. L. Shriner and D. Y. Curtin: *The Systematic Identification of Organic Compounds*
6. B. S. Roa and V. Deshpande: *Experimental Biochemistry*, I. K. Pvt. Ltd.
7. V. K. Ahluwalia and Renu Aggarwal: *Comprehensive Practical Organic Chemistry, Preparation and Qualitative Analysis*
8. Ghoshal, Mahapatra and Nad: *An Advanced Course in Practical Chemistry*.

SECOND SEMESTER

PAPER CODE: CHM T 421: PHYSICAL CHEMISTRY –II

(Quantum-, Statistical- Mechanics, Symmetry & GroupTheory)

Full Mark 100 (60 + 40)

Course Objectives: To learn the Important historic background of quantum mechanics versus classical mechanics, time-dependent and time-independent Schrödinger equations. Schrödinger wave equation in spherical coordinates, regid rotor. Basis functions and representation of orbital angular momentum operators and approximate methods of quantum mechanics. In addition, they should be able to know basic principles of atomic structure, term symbols and spectroscopic states, and principles and techniques of statistical thermodynamics.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 421.1]. Learn about the historic background of quantum mechanics versus classical mechanics.
[CHM T 421.2]. Understand the Schrödinger wave equation in spherical coordinates, rigid rotor.
[CHM T 421.3]. Understand the basic principles of atomic structure, term symbols and spectroscopic states.
[CHM T 421.4]. Able to learn the principles and techniques of statistical thermodynamics.
[CHM T 421.5]. Apply the concepts of symmetry and group theory and applications.

B. SYLLABUS

Unit – 1: Quantum Chemistry – I

***Historic Background*:** Important historic background of quantum mechanics versus classical mechanics, wave particle duality, Heisenberg's uncertainty principle.
***Schrödinger Wave Equation*:** normalization and orthogonality of wave functions; time-dependent and time-independent Schrödinger equations.

***Operators*:** Operators and their algebra, linear and Hermitian operators, matrix representation, commutation relationship, quantum mechanical operators for position, linear momentum, angular momentum, total energy, eigenfunctions, eigenvalues and eigenvalue equation; expansion of arbitrary state in term of complete set, postulates of quantum mechanics.
Solution of the Schrödinger Equations for Some Exactly Soluble Systems: particle-in-a-box; particle-in-a-ring and -sphere; harmonic oscillator; tunneling one dimensional potential barrier and well.

Unit – 2: Quantum Chemistry – II

Rigid Rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the phi equation, wave-function, quantum number, the theta equation, wave function, quantization of rotational energy, spherical harmonics.

***Hydrogen and Hydrogen Like Atoms*:** Radial and angular probability distributions, atomic orbitals.

***Angular Momentum*:** Basis functions and representation of orbital angular momentum operators, eigenfunctions, and eigenvalues of orbital angular momentum operator, Ladder operator, Spin, spin angular momenta, coupling (orbital and spin) of angular momentum, Clebsch-Gordan coefficients and Wigner Eckart theorem.

***Approximate Methods of Quantum Mechanics*:** Variational principle; time-independent perturbation theory up to second order in energy for non-degenerate and degenerate system with simple examples;

application to the two electron system such as, He and He like atoms.

Unit – 3: Atomic Structure and Spectroscopic

Many electron atoms, Pauli antisymmetry principle, Hund's rules; Slater determinant; Hatree and Hatree-Fock self consistent field model for atom; electronic term symbol (Russell-Saunders and jj coupling) for atoms and spectroscopic states (selection rules for atomic spectra).

Unit – 4: Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging; conical, grand conical and micro-canonical ensembles. Boltzmann distribution laws (using Lagrange's method of undetermined multipliers). Partition function – translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in term of partition function, Applications of partition functions.

Heat capacity behavior of solid – chemical equilibria and equilibrium constant in term of partition function. Fermi-Dirac statistics, distribution law and application to metal, Bose-Einstein statistics, distribution law and application to helium.

Unit – 5: Symmetry & Group Theory

symmetry elements and symmetry operations; point groups, Schoenflies notation for point group, representation of group by matrix, character of a representation, reducible and irreducible representation, great orthogonality theorem and its importance.

Application of group theory to atomic orbitals in ligand fields, molecular orbitals, and hybridization. Selection rules for IR and Raman spectra, procedure for determining symmetry of normal modes of vibration - hybrid orbitals in BF_3, CH_4, NH_3, H_2O and SF_6.

C. REFERENCE BOOKS:

1. Ira. N. Levine: *Quantum Chemistry*, Eds: 5th, PHI, 2000.
2. A. K. Chandra: *Introductory Quantum Chemistry*, Eds: 4th, Tata McGraw Hill, New Delhi, 1994.
3. P. Atkins and R. Friedman: *Molecular Quantum Mechanics*, Eds: 5th, Oxford University Press, 2011.
4. T. Engle and P. Reid: *Quantum Chemistry and Spectroscopy*, Pearson, New Delhi, 2011.
5. B. Widom: Statistical Mechanics: A Concise Introduction for Chemist, Cambridge University Press.
6. K. J. Laidler, *Chemical Kinetics*, Eds: 3rd, Pearson, 2011.
7. J Rajaram and J. C. Kuriacose: *Kinetics and Mechanisms of Chemical Transformations Applications of Femto-chemistry*, MacMillan, New Delhi, 2011.
8. F. A. Cotton, *Symmetry & Group Theory*.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSE	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 421.1	Learn about the historic background of quantum mechanics versus classical mechanics.	3		2				2	2			2
CHM T 421.2	Understand the Schrödinger wave equation in spherical coordinates, rigid rotor.	2	2				2		2	1		1
CHM T 421.3	Understand the basic principles of atomic structure, term symbols and spectroscopic states.	1			2		2				3	2
CHM T 421.4	Able to learn the principles and techniques of statistical thermodynamics.	2		1			2			2	2	2
CHM T 421.5	Apply the concepts of symmetry and group theory and applications.	2		1		3		2	2			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 422: INORGANIC CHEMISTRY –II

(Chemistry of Organometallics)

Full Mark 100 (60 + 40)

Course Objectives: The learners able to learn: To understand the basic concepts of organo transition metal chemistry, reactions, mechanism, and catalysis of organometallic complexes. Construction, structure and property of compounds with specific topology in organometallic chemistry. Understand the structure and bonding of inorganic rings, cages and clusters, and metal – ligand equilibria and stability of mononuclear, polynuclear and mixed ligand complexes in solution.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 422.1]. Understand the basic concepts of organo transition metal chemistry.
[CHM T 422.2]. Learn about the chemical reactions, mechanism, and catalysis of organometallic complexes.
[CHM T 422.3]. Learn about the structure and bonding of inorganic rings, cages and clusters.
[CHM T 422.4]. Provide insights into structure, property and applications of organometallic complexes.
[CHM T 422.5]. Understand the concepts of metal-ligand equilibria and stability of mixed ligand complexes.

B. SYLLABUS

Unit – 1: Organometallics – I

Organo transition metal chemistry: History, Nature of metal – carbon bonding and definition and classification of organometallic compounds, classification ligands, kinetic and thermodynamic stability of organometallic compounds. Compounds with metal carbon σ and multiple bond: Heptacity complexes of Metal-alkyl, -allyl, aryl, -carbene (Fischer and Schrock type), -carbonyl, -carbines and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity and decomposition pathway, Reactions in organometallic compounds. Stucture and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_2H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, techniques of study.

Unit – 2: **Organometallics – II**

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Catalysis by organometallic compounds: Hydrogenation of olefins, Wilkinson's catalyst, Tolman catalytic loop; synthesis gas, water-gas shift reaction; Hydroformylation (oxo process), Monsanto acetic acid process, Wacker process; synthetic gasoline: Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkens and alkynes, Zieglar- Natta catalysis, photo dehydrogenation catalyst (platinum POP).

Unit – 3: Inorganic Rings, Cages and Clusters

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds- Lipscomb's topological models, Wade`s rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

Unit – 4: New Developments in Organometallics Chemistry Research

Construction, structure and property of compounds with specific topology in Organometallic Chemistry: Capsules, boxes, containers, prisms or clusters, tubes, catenanes, rotaxanes, incorporation of metal atoms through metal-ligand coordination interactions, Various organic ligands containing carboxy, imidazole or pyridine groups, which can coordinate with metal atoms, have been used to generate the desired compounds (V, Cr, Mn, Fe, Co, Ni, Cu). Particularly, flexible ligands with central aromatic core and imidazol-1-ylmethyl pendant arms, e.g. 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene and its analogues, Interesting properties: olecular recognition, ion inclusion and exchange of these compounds, especially of the cage-like compounds, are described.

Unit – 5: Metal – ligand equilibria in solution

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic and template effect. Spectrophotometric and pH metric determination of binary formation constants.

C. Reference Books:

1. J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4th Pearson, New Delhi, 2006.
2. F. A Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann: *Advanced Inorganic Chemistry*, Eds: 6th, Wiley-India, New Delhi, 2010.
3. D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
4. Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
5. Robert Crabtree: *The Organometallic Chemistry of the Transition Metals*, 3rd Edition, Wiley.
6. Collman, Hegedus, Norton and Finke: *The Principles and Applications of Transition Metal Chemistry*, 2nd Eds, University Science Books.
7. Christoph Elschenbroich: *Organometallics*, 3rd Edition,
8. Wei-Yin Sun, *New Developments in Organometallics Chemistry***,** Wiley

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 422.1	Understand the basic concepts of organo transition metal chemistry.	2					1	2		1		2
CHM T 422.2	Learn about the chemical reactions, mechanism, and catalysis of organometallic complexes.	2		3			1	2	2	1		2
CHM T 422.3	Learn about the structure and bonding of inorganic rings, cages and clusters.	2	2	2	3	1			2			1
CHM T 422.4	Provide insights into structure, property and applications of organometallic complexes.	1	1						2			3
CHM T 422.5	Understand the concepts of metal-ligand equilibria and stability of mixed ligand complexes.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 423: ORGANIC CHEMISTRY –I I

(Principle of Organic Synthesis and Organic Spectroscopy)

Full Mark 100 (60 + 40)

Course Objectives: To learn the basic principles of organic synthesis and acid base catalyzed reactions, rearrangement and organometallic reactions. Understand the Ultraviolet and Infrared, NMR Spectroscopy analysis of organic compounds. Structure determination involving individual or combined use of the above spectral techniques

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 423.1]. Understand the basic principles of organic synthesis and acid base catalyzed reactions.
[CHM T 423.2]. Learn about rearrangement and organometallic and organic reactions.
[CHM T 423.3]. Understand the symmetry properties, stereoisomerism and stereospecific reactions.
[CHM T 423.4]. Learn the Understand the UV, IR, and NMR spectroscopy analysis of organic compounds.
[CHM T 423.5]. Understand the structure determination by using the UV, IR, and NMR spectral techniques

B. SYLLABUS

Unit – 1: Principles of Organic Synthesis

***Acid Catalyzed Carbon-Carbon Bond Formation Reaction*:** Principles, Self condensation of alkenes, reactions of aldehydes and ketones, Friedel-Crafts reactions, Prins reaction and Maanich reaction and Nef Reaction.
***Base Catalyzed Reactions* (*Enolate Chemistry*):** Enolates: structure and stability of enolates, Generation of enolates using Nucleophilic and non Nucleophilic bases. Kinetic and Thermodynamic control of regioselectivity of enolates, Reactions of enolates. Alkylation and acylation of enolates: Haloform reaction, HVZ reaction, Claisen condensation, Enolate of active methylene compounds and corresponding alkylation reactions, Michael addition, Robinson annulations reaction.

Unit – 2: Rearrangement and Organometallic Reactions

***Rearrangement Reactions*:** Demjanov, Pummerer, Dienone-phenol rearrangement, Pinacol-Pinacolone rearrangement, Fries rearrangement,Wagner-Meerwein Rearrangement, Benzil-Benzilic Acid Rearrangement, Beckmann Reaction, Curtius, Schmidt, Lossen, Hoffman and Claisen rearrangement. Brook, Favorski, Neber, Von Richter, Sommelet Hauser and Wittig rearrangement.
***Organometallic Reagents*:** Organomagnesium and Lithium reagents (Preparations, uses and applications), uses of Organomercury, organocadmium, organozinc and organocopper compounds.

Unit – 3: Ultraviolet and Infrared Spectroscopy

***Ultraviolet Spectroscopy*:** Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, solvent polarity. Calculation of absorption maxima by Woodward-Fieser Rules (using Woodward-Fieser tables for values for substituent's) for the following classes of organic compounds: conjugated polyenes (cyclic and acyclic), enones and substituted benzene derivatives.

***Infrared Spectroscopy*:** Fundamental, overtone and combination bands, vibrational coupling, important

group frequencies for the common functional groups.

Unit – 4: Nuclear Magnetic Resonance and Mass Spectroscopy

***Nuclear Magnetic Resonance Spectroscopy*:** Chemical shift, Factors affecting chemical shift, Chemical and magnetic equivalence, Spin-spin coupling, Coupling constant J, Factors affecting J, Karplus equation, First order spectra, Geminal, vicinal and long range coupling (allylic and aromatic). ^{13}C NMR, Heteronuclear coupling, 2D NMR spectroscopy.

***Mass Spectrometry*:** Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.

Unit – 5: Structure Determination of Organic Compounds

Structure determination involving individual or combined use of the above spectral techniques.

C. Reference Books:

1. J. Clayden, N. Greeves, S. Warren and P. Wothers: *Organic Chemistry*, Oxford
2. A. Carey and R.J. Sundberg: *Advance Organic Chemistry* (Part B).
3. Parikh, Parikh and Parikh: *Name reactions in Organic Synthesis*, Foundation Books, 2006.
4. G. Brahmachari: *Organic Name Reactions*, Narosa Publishers, 2009.
5. J. J. Li: *Name reactions in organic synthesis*, 3rd Edition, SPRINGER 2006.
6. Bessler and Silverstein: *Spectroscopy of Organic Compounds*, JOHN WILEY, 2001.
7. D. C. Pavia, G. M. Lampman, G. S. Kriz: *Introduction to Spectroscopy*, 3rd Edition, Thomson, 2007.
8. William Kemp: *Organic Spectroscopy,* III Edition

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 423.1	Understand the basic principles of organic synthesis and acid base catalyzed reactions.	2					1	2		1		2
CHM T 423.2	Learn about rearrangement and organometallic and organic reactions.	2		3			1	2	2	1		2
CHM T 423.3	Understand the symmetry properties, stereoisomerism and stereospecific reactions.	2	2	2	3	1			2			1
CHM T 423.4	Learn the Understand the UV, IR, and NMR spectroscopy analysis of organic compounds.	1	1						2			3
CHM T 423.5	Understand the structure determination by using the UV, IR, and NMR spectral techniques.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM P 421: PHYSICAL CHEMISTRY PRACTICAL – I

Full Mark 50

Course Objectives: The learners should be able to: Apply principles of kinetics of chemical reaction, determination of CMC, spectrophotometric determination of acid dissociation constant.

A. SYLLABUS

(i) Chemical Kinetics
- (a) Kinetics of Reaction between ferric nitrate and potassium iodide using initial reaction rates.
- (b) Determination of the rate constant for the decomposition of hydrogen peroxide by Fe^{3+} and Cu^{2+} ions.
- (c) Flowing clock reactions (Experiments in physical Chemistry by Shoemaker).

(ii) Determination of CMC of the surfactant/CMC Concentration.

(iii) Determination of partial molal volume.

(iv) Determination of the isotherm for a three component system.

(v) (a) Spectrophotometric determination of acid dissociation constant.
(b) Formula and stability constant using spectrophotometry.

B. Reference Books:

1. A. M. James and F. E. Prichard: *Practical Physical Chemistry*, Longman.
2. B. P. Levi: *Findley's Practical Physical Chemistry*,
3. R. C. Das and B. Behera: *Experimental Physical Chemistry*, Tata McGraw Hill.
4. D. P. Shoemaker, G. W. Garland and J. W. Niber: *Experimental Physical chemistry*, Mc Graw Hill Interscience.
5. A. J. Elias: *A collection of Interesting General Chemistry Experiments*, University Press, India.
6. J. Rose: *Advanced Physico-Chemical Experiments*, Sir Isaac Pitman & Sons Ltd, London.
7. J. B. Yadav: *Advanced Practical Physical Chemistry*, Krishna Prakashan Media (P) Ltd. Meerut.
8. P. C. Comboj: *University Practical Chemistry*, Vishal Publishing Co. Jalandhar.

PAPER CODE: CHM P 422: ORGANIC CHEMISTRY PRACTICAL - II

Full Mark 50

Course Objectives: The learners should be able to: Understand the multi-step organic synthesis involving the concept of protecting groups and selectivity in organic reaction and natural product extraction. Learners can monitor chemical reactions by using chromatographic techniques and synthesized organic compounds characterize by using IR, UV, NMR, and Mass spectroscopic techniques.

A. SYLLABUS

Part A: Multi Step Synthesis of Organic Compounds

Multi step organic synthesis involving the concept of protecting groups and selectivity in organic reaction. A Student must be involved to check TLC for monitoring the reaction progress and doing column chromatography for purification.

Characterization of synthesized organic compoundsusing IR, UV and NMR, and mass spectroscopic techniques are to be studied.

- Nitrobenzene→aniline→Acetanilide (Nitration and followed by reduction)
- Malonic acid→cinnamic acid→methyl cinnamate (Condensation reaction and next followed by esterification)
- Benzaldehyde→benzoin→benzil→benzilic acid (Umpolung strategy, Oxidation reaction and next benzylic acid rearrangement reaction)
- Aniline→benzenediazonium chloride→benzeneazo-2-naphthol (Azodye synthesis)
- Skraup's synthesis: Quinoline from *o*-aminophenol (Heterocyclic compound synthesis)
- Acetanilide→p-acetamidobenzenesulfonylchloride→p-acetamidobenzenesulfonamide→sulfanilamide (Sulfa Drug synthesis)
- cinnamaldehyde→cinnamyl alcohol→cinnamyl bromide→allyl-aryl ether synthesis (Nucleophilic substitution reaction)

Part B: Extraction Method

- **Natural product extraction:** Solasidine, Caffeine, Nicotine, Peptine, Rosine, Carotenoids, Computational methods of retro-synthetic analysis modeling and calculation.

B. Reference Books:

1. A. I. Vogel: *Practical Organic Chemistry*
2. F. G. Mann and B. C. Saunders: *Practical Organic Chemistry*
3. J. Leonard, B. Lygo and G. Proctor: *Advanced Practical Organic Chemistry*
4. Addison Ault; *Techniques and Experiments for Organic Chemistry*, University Science Book
5. R. L. Shriner and D. Y. Curtin: *The Systematic Identification of Organic Compounds*
6. B. S. Roa and V. Deshpande: *Experimental Biochemistry*, I. K. Pvt. Ltd.
7. V. K. Ahluwalia and Renu Aggarwal: *Comprehensive Practical Organic Chemistry, Preparation and Qualitative Analysis*
8. Nad, Mahapatra and Ghoshal: *An Advanced Course in Practical Chemistry*

SEMESTER – III

PAPER CODE: CHM T 511: PHYSICAL CHEMISTRY-III

(Chemical Bonding, Non-equilibrium Thermodynamics and Solid State Chemistry)

Full Mark 50 (60 + 40)

Course Objectives: The learners should be able to apply basic principles of chemical bonding in diatomic molecules and concepts of MO and VB theories. The course will also provide Ab-initio methods for closed shell systems, Koopman's and Hellman-Feynman theorems. Learn about the concepts of laws, and open systems and non-ideal system of thermodynamics and non-equilibrium thermodynamics. Solid state chemistry, crystals defects and magnetic properties

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 511.1]. Understand the chemical bonding in diatomic molecules and elementary concepts of MO and VB theories.

[CHM T 511.2]. Introductory of semi-empirical and *ab-initio* calculations on molecular systems.

[CHM T 511.3]. Concepts of thermodynamics laws and open and non-ideal system thermodynamics.

[CHM T 511.4]. Apply concepts on thermodynamic criteria for non-equilibrium states.

[CHM T 511.5]. Understand the Solid state chemistry, crystals defects and magnetic properties.

B. SYLLABUS

Unit – 1: Molecular Structure

Chemical bonding in diatomic; elementary concepts of MO and VB theories; Born-Oppenheimer approximation, MO treatment for H_2^+ ion, MO treatment of homo- and hetero- nuclear diatomic molecules; comparison of MO and VB theories. Hückel MO theory for conjugated π-systems. Polyatomic molecules, hybridisation and valence MOs of simple molecule like H_2O, NH_3, CH_4, C_2H_6 *etc*.

Unit – 2*: Ab-initio* Methods for Closed Shell Systems

Introductory treatment of semi-empirical and *ab-initio* calculations on molecular systems; the Hartree-Fock Self-Consistent Field Method; the generation of optimized orbitals, Koopman's theorem (The Physical Significance of Orbital Energies), electron correlation energy; density matrix analysis of the Hartree-Fock approximation, natural orbitals, matrix solution of the Hartree-Fock equations (Roothaan's equations); Hellman-Feynman theorem.

Unit – 3: Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential, and entropies. Thermodynamics of open systems: partial molal properties, partial molal free energy, partial molal volume and partial molal heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity.

Non-ideal system: excess function for non ideal solutions. Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solution; determination of activity and activity coefficients; ionic strength.

Unit – 4: Non-equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium state, entropy production and entropy flow, energy balance equation for different irreversible processes (e.g. heat flow, chemical reaction etc.), transformation of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equation, microscopic, reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological system, coupled reactions.

Unit – 5: Solid State Chemistry

Perfect and imperfect crystals, intrinsic and extrinsic defect, point defect, line and plane defect, vacancies, Schottky and Frankel defects; thermodynamics of Schottky and Frankel defect formation, color center, non-stochiometry defects. Metal insulators and semiconductors, electronic structure of solids-band theory, band structure of metals, insulators and semi-conductors, doping semi-conductors, *p-n* junction; superconductors; photoelectric effects; magnetic properties. Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

C. Reference Books:

1. Ira. N. Levine: Quantum Chemistry, Eds: 5th, PHI, 2000.
2. A. K. Chandra: *Introductory Quantum Chemistry*, Eds: 4th, Tata McGraw Hill, New Delhi, 1994.
3. P. Atkins and R. Friedman: *Molecular Quantum Mechanics*, Eds: 5th, Oxford University Press, 2011.
4. T. Engle and P. Reid: *Quantum Chemistry and Spectroscopy*, Pearson, New Delhi, 2011.
5. B. R. Puri, L. R. Sharma and M. S. Pathania, *Principle of Physical Chemistry*, Eds. 44th, Vishal Publishing Co., Jalandhar, 2010.
6. P. Atkins and J. D. Paula, *Physical Chemistry*, Eds. 7th, Oxford University Press, New Delhi, 2002.
7. R. S. Berry, S. A. Rice and J. Ross: P*hysical Chemistry*, Eds: 2nd, Oxford University Press, New Delhi, 2007.
8. S. R. Degroot, P. Mazur: *Non-Equilibrium Thermodynamics*, North Holland Publication, Amsterdam, 1961.
9. C. N. R. Rao and J. Gopalakrishnan: *New Direction in Solid State Chemistry*, Cambridge University Press, 1997.
10. A. R. West: *Solid State Chemistry and Its Applications,* John Wiley & Sons, 1989.
11. L. Smart and E. Moore: *Solid State Chemistry*, Chapman and Hall, 1992.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 511.1	Understand the chemical bonding in diatomic molecules and elementary concepts of MO and VB theories.	2					1	2		1		2
CHM T 511.2	Introductory of semi-empirical and *ab-initio* calculations on molecular systems.	2		3			1	2	2	1		2
CHM T 511.3	Concepts of thermodynamics laws and open and non-ideal system thermodynamics.	2	2	2	3	1			2			1
CHM T 511.4	Apply concepts on thermodynamic criteria for non-equilibrium states..	1	1						2			3
CHM T 511.5	Understand the Solid state chemistry, crystals defects and magnetic properties.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation Substantial Correlation

PAPER CODE: CHM T 512: INORGANIC CHEMISTRY –III

(Bio-Inorganic & Nuclear Chemistry)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basic importance, structure, bonding and mechanism of primary and advanced bio-inorganic chemistry in daily life. To learn the metallic enzymes, carbonic anhydrase, xanthine oxidase, aldehyde oxidase and etc. To get the insights and concepts of introduction of inorganic photochemistry, photophysical and photochemical process along with nuclear chemistry & radiochemical analysis.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 512.1]. Learn the basic structure, bonding advanced bio-inorganic chemistry in daily life.
[CHM T 512.2]. Learn about basic properties of metallic enzymes, carbonic anhydrase and etc.
[CHM T 512.3]. Learn about the magnetic properties of transition series metals, lanthanides and actinides.
[CHM T 512.4]. Understand the basic concepts introduction of inorganic photochemistry, photophysical and photochemical process.
[CHM T 512.5]. Learn the nuclear chemistry & radiochemical analysis in inorganic compounds.

B. SYLLABUS

Unit – 1: Bio-inorganic Chemistry – I

Transport and storage of dioxygen: Active site structures and bio functions of O_2-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes. Chelato theraphy. Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome *c*; iron-sulfur proteins (rubredoxin, ferredoxines), organic-redox protein cofactors – FAD, NAD, FMN, ubiquinone; blue copper proteins, HIPIP. Respiratory electron transport chain, cytochrome c oxidase. Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and abiological nitrogen fixing systems, model study.

Unit – 2: Advanced Bio-inorganic Chemistry – II

Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer.

Redox enzymes: Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450,

Nitrogen cycle enzymes: NO*x* reductases, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase, sulfite oxidase, xanthine oxidase, nitrogenase, P and M clusters in nitrogenase, transition metal dinitrogen complexes and insights into N_2 binding, reduction to ammonia.

Unit – 3: Enzymes

Zinc enzymes, magnesium enzymes, iron enzymes, carbonic anhydrase, xanthine oxidase, aldehyde oxidase, cobalt containing enzymes, Mo and tungsten enzymes, Vitamin B-12
***Zinc in Transcription*:** Zinc fingers, zinc thiolate clusters.
***Calcium Signaling Protein*:** Calmodulin protein and Ca^{2+} ion pump
***Biological Cycle*:** Nitrogen cycle, hydrogen cycle, in vivo and vitro nitrogen fixation
***Sensors*:** Iron protein as sensor, Copper sensor, protein that sense copper and zinc level

***Other Application*:** Biominiralization, cancer treatment, antiarthristis drugs
Contribution of Individual Elements in Biological Function: Na, K, Li, Mg, Ca, Se, Mn, Fe, Co, Ni, Cu, Zn, Mo, W, Si, Pt, Au.

Unit – 4: Inorganic Photochemistry

Introduction to inorganic photochemistry, photophysical and photochemical process. Excitation modes in transition metal complexes, fate of photo-excited species, fluorescence and phosphorescence applied to Inorganic systems, intramolecular energy transfer, vibrational relaxation, internal conversion and intrasystem crossing, quantum yield, decay fluorescence. Fluorence quenching, Stern-Volmer equation. Photochemical process: photo substitution and photoelectron transfer reactions in Co, Cr, Ru and Rh complexes.

Unit – 5: Nuclear Chemistry & Radiochemical Analysis

Nuclear models: **N**uclear stability, terrestrial abundance and distribution, relativistic effect, electronic configuration, oxidation states, aqueous-, redox- and complex- chemistry; Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism. *Nuclear reactions:* Energetics, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), Nuclear reactors and particle accelerators.

Radioactive Techniques: Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

C. References Books:

1. S. J. Lippard and J. M. Berg: *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, 1994.
2. W. Kaim and B. Schwederski: *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley & Sons Inc., 1994.
3. D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
4. B. R. Puri, L. R. Sharma, and K. C. Kalia: *Principle of Inorganic Chemistry*, Milestone Publisher, New Delhi **2010**.
5. D. L. Nelson, & M. M. Cox: *Lehninger's Principles of Bioch*emistry *7 Ed.,* W. H. Freeman
6. H. J. Arnikar, Essential of Nuclear Chemistry, Wiley-Blackwell; 2nd Edition edition.
7. *Hand Book of Nuclear Reactions*, edited by **Vértes,** A., **Nagy**, S., **Klencsár,** Z., **Lovas,** R.G., **Rösch,** F. , Springer
8. J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4th Pearson, New Delhi, 2006.
9. A. Das and G. N. Mukherjee, Elements of Boi-inorganic Chemistry.
10. Ashim Kr. Das, Boi-inorganic Chemistry.


AMARKANTAK (M.P.)
विद्यया विन्दतेऽखिलम्

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 512.1	Learn the basic structure, bonding advanced bio-inorganic chemistry in daily life.	2					1	2		1		2
CHM T 512.2	Learn about basic properties of metallic enzymes, carbonic anhydrase and etc.	2		3			1	2	2	1		2
CHM T 512.3	Learn about the magnetic properties of transition series metals, lanthanides and actinides.	2	2	2	3	1			2			1
CHM T 512.4	Understand the basic concepts introduction of inorganic photochemistry, photophysical and photochemical process.	1	1						2			3
CHM T 512.5	Learn the nuclear chemistry & radiochemical analysis in inorganic compounds.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 513: ORGANIC CHEMISTRY –III

(Pericyclic Reaction, Photochemistry and Free Radical Chemistry)

Full Mark 100 (60 + 40)

Course Objectives: The learners able to: Learn the basic introduction of pericyclic reaction and electrocyclic and cycloaddition reactions of pericyclic compounds. Understand the classification of sigmatropic rearrangement reaction and mechanism, Learn the basic principle of photochemistry and reaction with carbonyl compounds, photo reduction, and photo isomerization reactions and free radical reactions.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 513.1]. Understand the basic introduction of pericyclic reactions.
[CHM T 513.2]. Learn about the electrocyclic and cycloaddition reactions of pericyclic compounds.
[CHM T 513.3]. Learn about the classification of sigmatropic rearrangement reaction and mechanism.
[CHM T 513.4]. Apply concepts on photochemistry and reaction with carbonyl compounds.
[CHM T 513.5]. Understand the photo isomerization reactions and free radical reactions.

B. SYLLABUS

Unit – 1: Introduction of Pericyclic Reaction

Definition, Symmetry of π molecular orbital, Filling of electrons in π molecular orbital in conjugated polyenes, conjugated ions, Frontier Molecular Orbital Theory, Classification of Pericyclic reactions

Unit – 2: Electrocyclic and Cycloaddition Reactions

***Electrocyclic Reactions*:** Conrotatory and disrotatory motion in ring opening and ring closing reactions, Frontier Molecular Orbital (FMO) approach for Electrocyclic reactions, Correlation diagram of the Electrocyclic reactions with 4nπ and (4n + 2)π electronic systems, Woodward – Hoffmann rule for Electrocyclic system.

***Cycloaddition Reactions*:** Theory of Cycloaddition reaction, Stereochemistry of Cycloaddition reaction, Diels-Alder reaction, 1, 3-Dipolar Cycloaddition reactions, Chelotropic reactions. Woodward – Hoffmann selection rule for Electrocyclic system.

Unit – 3: Sigmatropic Rearrangement and Group Transfer Reactions

Definition, Classification of Sigmatropic Rearrangement, Mechanism of Sigmatropic Rearrangement, Various types of [m, n] Sigmatropic rearrangements, Cope, Oxy-Cope and Claisen Rearrangement. Ene Reactions and Group Transfer Reactions given by Diimide.

Unit – 4: Photochemistry

***Basic Principle of Photochemistry and Reaction with Carbonyl compounds*:** Introduction of Photochemistry-Jablonski Diagram, Quantum Yield calculation of photo chemical reaction, photosensitizer and quencher; α-cleavage (Norrish type I & II) and β-cleavage reactions with carbonyl compounds, Intra- and Intermolecular Hydrogen abstraction reactions with carbonyl compounds, Photocycloaddition reactions (Paterno-Bűchi Reaction).

***Photo Rearrangement, Photo Reduction, and Photo Isomerization Reactions*:** Di- π-Methane Rearrangement, Aza-di- π-Methane Rearrangement, Photo reduction of carbonyl compounds, Cis-Trans Isomerization reactions with alkenes, Photochemistry of Dienes.

Unit – 5: Free Radical Reactions

Principles, Generation of free radicals, Formation of Carbon-Halogen bonds (Hundsdiecker reaction), Formation of Carbon-Carbon bonds (addition to carbon-carbon double bonds, Acyloin condensation reaction, Eglinton reaction). Formation of Carbon-Nitrogen bonds (Barton Recation and Hoffmann-Loeffler-Freytag Reaction).

Reference Books:

1. J. Singh & J. Singh: *Photochemistry and Pericyclic Reactions*, New Age International (P) Ltd., 2007
2. B. B. Woodward and Hoffman: *Conservation of Orbital Symmetry*, Verlag Chemie Academic Press, 1971.
3. W. Carruthers: *Some Modern Methods of Organic Synthesis*, Cambridge University, Press, 1993.

C. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 513.1	Understand the basic introduction of pericyclic reactions	2					1	2		1		2
CHM T 513.2	Learn about the electrocyclic and cycloaddition reactions of pericyclic compounds.	2		3			1	2	2	1		2
CHM T 513.3	Learn about the classification of sigmatropic rearrangement reaction and mechanism.	2	2	2	3	1			2			1
CHM T 513.4	Apply concepts on photochemistry and reaction with carbonyl compounds.	1	1						2			3
CHM T 513.5	Understand the photo isomerization reactions and free radical reactions.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM P 511: PHYSICAL CHEMISTRY PRACTICAL – II

Course Objectives: The learners should be able to: Understand the principles and applications of conductometry, ptitrations, potentiometry/pHmetry, polarizability, IR and Raman spectroscopy of the solvent mixtures.

A. SYLLABUS

(i) Conductometry

(a) The measurement of electrical conductance for the determination of the equivalent conductance at infinite dilution.
(b) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulfate using Debye-Hückel's limiting law.
(c) To verify Debye-Hückel limiting law for strong electrolyte.

(ii) (a) Rate of the hydrolysis of sucrose using polarimeter.
(b) Polarizability from refractive index measurement.

(iii) Potentiometry/pHmetry
(a) Determination of pKa of poly-basic acid with the pH meter.
(b) To determine the pH of various mixtures of acetic acid and sodium acetate in aqueous solutions and hence determine the dissociation constant of the acid.

(iv) Determination of the transport number by moving boundary method.

(v) IR and Raman spectroscopy of the solvent mixture.

B. Reference Books:

1. A. M. James and F. E. Prichard: *Practical Physical Chemistry*, Longman.
2. B. P. Levi: *Findley's Practical Physical Chemistry*,
3. R. C. Das and B. Behera: *Experimental Physical Chemistry*, Tata McGraw Hill.
4. D. P. Shoemaker, G. W. Garland and J. W. Niber: *Experimental Physical chemistry*, Mc Graw Hill Interscience.
5. A. J. Elias: *A collection of Interesting General Chemistry Experiments*, University Press, India.
6. J. Rose: *Advanced Physico-Chemical Experiments*, Sir Isaac Pitman & Sons Ltd, London.
7. J. B. Yadav: *Advanced Practical Physical Chemistry*, Krishna Prakashan Media (P) Ltd. Meerut.

PAPER CODE: CHM P 512: INORGANIC CHEMISTRY PRACTICAL – II

Course Objectives: The learners should be able to: Understand the analysis of Ores, Soil samples by using Analytical techniques. The learners should be able to: Synthesize the inorganic compound (complex) and their studies by IR, Electronic spectra, Mössbauer and magnetic susceptibility measurements.

A. SYLLABUS

I. Analytical Chemistry:

- Analysis of Ores: Felspar , bauxite, Rocks available in that region.
- Analysis of Soil sample, animal feeds, soil micronutrients, milk powder for Ca, Fe and P content.
- Separation of Mixture: Chromium (III) and Mn(II) in a mixture, Iron (III) and Cu(II) in a mixture, Iron(III) and Al(III) in a mixture

At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session.

II. Preparations of Complex (At Least eight samples)

Preparation of selected inorganic compound and their studies by I.R. electronic spectra, Mössbauer and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds

1. bis(ethylene)nickel(II)thiosulphate,
2. tris(acetylacetonato)manganese(III), tris(acetylacetonato)Aluminium(III), tris(acetylacetonato)iron(II), tris(acetylacetonato)copper(II),
3. Hexaminecobalt(III)chloride,
4. Mercury tetrathiocyanatocobaltate(II),
5. Copper(II) biguanide
6. Mn_{12} Acetate Single Molecule Magnet
7. Preparation of copper glycine complex- cis and trans bis- (glycinato) copper (II).
8. Preparation of N, N-bis-(salicyldehyde) ethylenediamine, Co(salen), Mn(salen), determination of O_2 absorption by Co(salen), reaction of oxygen adduct with $CHCl_3$ (deoxygenation).
9. VO(*acac*)$_2$
10. *cis*-K $[Cr(C_2O_4)_2 (H_2O)_2]$
11. $Na[Cr(NH_3)_2 (SCN)_4]$
12. $K_2[Fe(C_2O_4)_3]$

C. Reference Books:

1. *Vogel's Textbook of Quantitative Analysis*, Revi Mendham, ELBS.
2. W.L. Jolly, *Synthesis and Characterization of Inorganic Compounds*, Prentice Hall.

SEMESTER – IV

PAPER CODE: CHM T 521: MOLECULAR SPECTROSCOPY

Full Mark 100 (60 + 40)

Course Objectives: To learn basic principles of Microwave, Vibrational (IR and Raman), Electronic spectra, NMR and Photoacoustic, and Mössbauer Spectroscopy and to use these spectroscopic methods for organic/inorganic structure elucidation.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 521.1]. Understand the basic principles and interaction of electromagnetic radiation with matter.
[CHM T 521.2]. Apply the concepts of microwave (rotational) spectroscopy techniques.
[CHM T 521.3]. Learn the basic principles and applications of vibrational (IR and Raman) spectroscopy.
[CHM T 521.4]. Learn the concepts of electronic (atomic, molecular, and photoelectron) spectroscopies.
[CHM T 521.5]. Understand the basic principles and applications of NMR and photoacoustic and mössbauer spectroscopy.

B. SYLLABUS

Unit – 1: Unifying Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarization, and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment selection rules, intensity of spectral line. Born-Oppenheimer approximation, rotational, vibrational, and electronic energy levels. Fourier Transform Spectroscopy.

Unit – 2: Microwave Spectroscopy

***Rotational spectroscopy*:** Classification of molecules, rigid rotor model, selection rule, intensity of spectral line, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect nuclear and electron spin interaction and effect of external field. Applications (determination of bond lengths of diatomic and linear triatomic molecules *etc*.)

Unit – 3: Vibrational Spectroscopy

A. *Infrared Spectroscopy*: Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R branches. Breakdown of Oppenheimer approximation; vibration of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factor affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis. Fourier Transform Infra-red Spectroscopy (FTIR).

B. *Raman Spectroscopy*: Classical and quantum theories of Raman Effect, pure rotational, vibrational, and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti-stokes Raman spectroscopy (CARS).

Unit – 4: Electronic Spectroscopy

A. *Atomic Spectroscopy*: Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

B. *Molecular Spectroscopy*: Energy levels, molecular orbitals, vibranic transition, vibrational progressions and geometry of excited state, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complex, charge transfer spectra.

C. *Photoelectron Spectroscopy*: Basic principle; photo-electronic effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA, basic idea Auger electron spectroscopy.

Unit – 5: Magnetic Resonance, Photoacoustic, and Mössbauer Spectroscopy

A. *Nuclear Magnetic Resonance Spectroscopy*: Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factor influencing chemical shift, deshielding, spin-spin interaction, factor influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc), spin decoupling; basic idea about instrument, NMR studies of nuclei other than proton – 13C, 19F, and 31P; FT NMR, advantage of FT NMR, use of NMR in medical diagnostics.

B. *Electron Spin Resonance Spectroscopy*: Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densityies and McConnell relationship, measurement techniques, applications.

C. *Nuclear Quadrupole Resonance Spectroscopy*: Quatrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

D. *Photoacoustic Spectroscopy*: Basic principles of photoacoustic spectroscopy (PAS). PAS-gases and condensed system, chemical and surface applications.

E. *Mössbauer Spectroscopy*: Basic principles, spectral parameters and spectrum display. Application of technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds – nature of M-L bond, coordination number, structure and (ii) detection of oxidation state and inequivalent MB atom.

C. Reference Books:

1. T. Engle and P. Reid: *Quantum Chemistry and Spectroscopy*, Pearson, New Delhi, 2011.
2. B. K. Sharma: *Instrumental Methods of Chemical Analysis* - 9th Edition.
3. William Kemp: *Organic Spectroscopy* –3rd Edition.
4. C. N. Banwell and E. M. McCash: *Fundamentals of Molecular Spectroscopy*, Ed. 4th, Tata McGraw-Hill, 1994.
5. G. M. Barrow: *Introduction to Molecular Spectroscopy*

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 521.1	Understand the basic principles and interaction of electromagnetic radiation with matter.	2					1	2		1		2
CHM T 521.2	Apply the concepts of microwave (rotational) spectroscopy techniques.	2		3			1	2	2	1		2
CHM T 521.3	Learn the basic principles and applications of vibrational (IR and Raman) spectroscopy.	2	2	2	3	1			2			1
CHM T 521.4	Learn the concepts of electronic (atomic, molecular, and photoelectron) spectroscopies.	1	1						2			3
CHM T 521.5	Understand the basic principles and applications of NMR and photoacoustic, and mössbauer spectroscopy.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation, Substantial Correlation

PAPER CODE: CHM P 522: PROJECT AND DISSERTATION

Each student is assigned to a faculty supervisor to carry out a research project. They will be trained in searching research literature as well as experimental and computational work specific to the chosen research problem. On the basis of partial fulfilment of project report the student may go other University/Institute for project work. At the end of the project they will submit a report of the work done and make a presentation for evaluations.

LIST OF ELECTIVE PAPER

S. No.	Course Code	Course Structure	Title of Paper	Credit
1	CHM T 601	Elective	Mathematics for Chemist	4
2	CHM T 602	Elective	Biology for Chemist	4
3	CHM T 603	Elective	Industrial Chemistry	4
4	CHM T 604	Elective	Instrumental Methods of Analysis	4
5	CHM T 605	Elective	Basic of Materials Chemistry	4
6	CHM T 606	Elective	Introduction to Nanomaterials and Nanotechnology	4
7	CHM T 607	Elective	Polymers Chemistry	4
8	CHM T 608	Elective	Bioorganic and Drug Chemistry	4
9	CHM T 609	Elective	Advanced Heterocyclic Chemistry	4
10	CHM T 610	Elective	Chemistry of Natural Products	4
12	CHM T 611	Elective	Solid State Chemistry	4
13	CHM T 612	Elective	Advanced Synthetic Organic Chemistry	4

PAPER CODE: CHM T 601: MATHEMATICS FOR CHEMIST (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the numbers: real and complex number, vectors: vectors, dot, cross and triple product etc. Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices) and their properties. Functions, continuity and differentiability, rules for differentiation, application of differential calculus including maxima and minima

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 601.1]. Understand the basics of Learn the numbers: real and complex number, vectors.
[CHM T 601.2]. Learn matrix algebra and addition and multiplication; inverse matrices.
[CHM T 601.3]. Learn about functions, continuity and differentiability, rules for differentiation.
[CHM T 601.4]. Understand the concepts of functions, continuity and differentiability and rules.
[CHM T 601.5]. Understand basics of permutation, combination, probability, stirling's approximation.

B. SYLLABUS

Unit – 1: Vectors and Matrix Algebra

***Numbers*:** Real and Complex number
***Vectors*:** Vectors, dot, cross and triple product etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem *etc*.

Unit – 2: *Matrix Algebra*

Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (symmetric, screw-symmetric, Hermitian, screw-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations; homogeneous, non-homogeneous linear equation and conditions for the solution, linear dependence and independence. Introduction of vector spaces, matrix eigenvalues and eigenvectors, digonalization, determinants (examples from Hückel theory). Introduction to tensors; poarizability and magnetic susceptibility as examples.

Unit – 3: Differential and Calculus

Differential: Functions, continuity and differentiability, rules for differentiation, application of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.), exact and inexact differentials with their application to the thermodynamic properties.

Partial Differential: Function of several variables, partial differentiation, co-ordinate transformation (e.g. Cartesian to spherical polar).
Integral calculus: basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus.

Unit – 4: Elementary Differential Equations

Ordinary first- and second-order differential equations. Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions. Numerical solutions. Special functions: Hermite, Legendre and Laguerre polynomials, recursion relations.

Unit – 5: Probability and Curve Sketching

Permutation & Combination. Probability. Stirling's approximation. Lagrange multipliers. Curve sketching and curve fitting; Introduction to Fourier series and Fourier transforms.

C. Reference Books:

1. R. G. Mortimer: *Mathematics for Physical Chemistry*, Academic Press.
2. F. Diniels: *Mathematical Preparation for Physical chemistry*, McGraw Hill.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 601.1	Understand the basics of Learn the numbers: real and complex number, vectors.	2					1	2		1		2
CHM T 601.2	Learn matrix algebra and addition and multiplication; inverse matrices.	2		3			1	2	2	1		2
CHM T 601.3	Learn about functions, continuity and differentiability, rules for differentiation.	2	2	2	3	1			2			1
CHM T 601.4	Understand the concepts of functions, continuity and differentiability and rules.	1	1						2			3
CHM T 601.5	Understand basics of permutation, combination, probability, stirling's approximation	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 602: BIOLOGY FOR CHEMIST (ELECTIVE)

(Biology for Chemist)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the structure and functions of prokaryotic and eukaryotic cells, intracellular organelles and also the structure and functions of important derivatives of monosaccharides, fatty acids and essential fatty acids. Understand the chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of protein and nucleic acids.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 602.1]. Learn the structure and functions of prokaryotic and eukaryotic cells, intracellular organelles.

[CHM T 602.2]. Learn about the structure and functions of important derivatives of monosaccharides.

[CHM T 602.3]. Understand the concepts and functions fatty acids and essential fatty acids**.**

[CHM T 602.4]. Understand the concepts of chemical and enzymatic hydrolysis of proteins to peptides.

[CHM T 602.5]. Understand the purine and pyrimidine bases of nucleic acids, base pairing via H-bonding.

B. SYLLABUS

Unit – 1: Cell Structure & Functions

Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism; ATP the biological energy currency. Origin of life – unique property of carbon, chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-molecules.

Unit – 2: Carbohydrates

Conformation of monosaccharides, structure and function of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinsitol, amino sugars, N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose, and chitin; storage polysaccharides – starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins glycolipids. Role of sugar in biological recognition. Blood group substances. Ascorbic acid, carbohydrate metabolism – Krebs' cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis pentose phosphate pathway.

Unit – 3: Lipids

Fatty acids, essential fatty acids, structure and function of triglycerols; glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins – composition and function, role in atherosclerosis. Properties of lipids, aggregates – micelles, bilayers, liposomes and their possible biological function. Biological membranes, fluid mosaic model of membranes structure. Lipid metabolism □-oxidation of fatty acids.

Unit – 4: Amino Acids

***Amino Acids, Peptides and Proteins*:** Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, force responsible for holding of secondary structure. □-helix, □-sheet, super secondary structure, triple helix structure of collagen. Tertiary structure of proteins, folding and domain structure. Quaternary structure. Amino acid metabolism, degradation and biosynthesis of amino acids,

sequence determination, chemical/enzymatic/mass spectral racemization detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

Unit – 5: Nucleic Acids

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis of heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono- and tri-nucleosides.

C. Reference Books:

1. A. L. Lehninger: *Principle of Biochemistry*, Worth Pub. Shers.
2. L. Stryer and W. H. Freeman, *Biochemistry*
3. J. David Rawn: *Biochemistry*, Neil Patterson.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 602.1	Learn the structure and functions of prokaryotic and eukaryotic cells, intracellular organelles.	2					1	2		1		2
CHM T 602.2	Learn about the structure and functions of important derivatives of monosaccharides.	2		3			1	2	2	1		2
CHM T 602.3	Understand the concepts and functions fatty acids and essential fatty acids**.**	2	2	2	3	1			2			1
CHM T 602.4	Understand the concepts of chemical and enzymatic hydrolysis of proteins to peptides.	1	1						2			3
CHM T 602.5	Understand the purine and pyrimidine bases of nucleic acids, base pairing via H-bonding.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 603: INDUSTRIAL CHEMISTRY (ELECTIVE)
Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the water and its treatment and water analysis. Basics of physical and chemical properties and manufacturing of glass and rubber. Concepts of fertilization, nitrogeneous fertilizers, method of production and its action and classification. Learn the classification of petroleum compounds and their thermal cracking, hydrocracking, and fluid catalytic cracking. Preparation and application of synthetic fibers and dyes and dyeing.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 603.1]. Understand the concepts of water and its treatment and water analysis.
[CHM T 603.2]. Learn about the physical and chemical properties and manufacturing of glass and rubber.
[CHM T 603.3]. Concepts of method of production and its action of fertilization, nitrogeneous fertilizers.
[CHM T 603.4]. Understand the nature of petroleum compounds and their thermal cracking, hydrocracking, and fluid catalytic cracking.
[CHM T 603.5]. Learn the preparation and applications of synthetic fibers and dyes and dyeing.

B. SYLLABUS

Unit – 1: Water and Its Treatment

Sources of water, chlorinated and nonchlorinated water, chemical method of sterilization: precipitation method, Aeration, ozonisation, chlorination, chloramines process, potassium permanganate method, Physical method of sterilization: Boiling, exposure to sunlight, hard and soft water, Types of hardness, temporary and permanent hardness, water softening, cold and hot lime soda process, zeolite process, ion exchange process, removal of iron, silica, and dissolved oxygen from water for industrial purposes, water for boiler uses, water analysis.

Unit – 2: Glass and Rubbers

***Glass*:** physical and chemical properties of glass, constituents in glasses, raw materials, manufacturing of glasses, optical glass, borosilicate glass, lead glass, colored glass, opal glass, safety glass, fiber glass.
***Natural and Synthetic Rubber*:** classification of rubber, natural and synthetic rubber.

Unit – 3: Chemical Fertilizers

Classification of fertilization, nitrogeneous fertilizers, method of production and its action- ammonium nitrate, ammonium sulphate, urea, calcium cyanamide, ammonium chloride, phosphate rock, normal super phosphate, triple super phosphate.

Unit – 4: Petroleum

Classification of petroleum, composition of petroleum, mining of petroleum, refining of petroleum, octane rating, octane number and antiknock compound, cetane number, production of gases, crude naptha, benzene, kerosene oil, fuel oil, lubricating oil, paraffin wax and black tarry after refining. Cracking: thermal cracking, hydrocracking, and fluid catalytic cracking.

Unit – 5: Fibers and Dyes

***Synthetic Fibers*:** Preparation of fibers- Nylons, Nylon-66, Nylon-6, Nylon-11, Nylon-610, Nylon-8, polyethylene terephthalate, orlon, saran, vinyon, taflon.
S*ynthetic Dyes and Dyeing*: Requisites of true dyes, sensation of color, witt's theory, chromophores, auxochromes: batho-, hypso-, hyper-, and hypochromic shifts; classification of dyes: acid dyes, basic dyes, adjective dyes, vat dyes, ingrain dyes, sulfur dyes, pigment dyes, nitroso dyes, nitro dyes, azo dyes, xanthenes dyes, applications of dye.

C. Reference Books:

1. E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
2. R.M. Felder, R.W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
3. J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
4. S. S. Dara: *A Textbook of Engineering Chemistry*, S. Chand & Company Ltd. New Delhi.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 603.1	Understand the concepts of water and its treatment and water analysis.	2					1	2		1		2
CHM T 603.2	Learn about the physical and chemical properties and manufacturing of glass and rubber.	2		3			1	2	2	1		2
CHM T 603.3	Concepts of method of production and its action of fertilization, nitrogeneous fertilizers.	2	2	2	3	1			2			1
CHM T 603.4	Understand the nature of petroleum compounds and their thermal cracking, hydrocracking, and fluid catalytic cracking.	1	1						2			3
CHM T 603.5	Learn the preparation and applications of synthetic fibers and dyes and dyeing.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 604: INSTRUMENTAL METHODS OF ANALYSIS (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners should be Able to: Learn the basic principles, instrumentation, techniques and applications of UV-Vis, Fluorescence, FI-IR and Raman spectroscopy. Understand the atomic absorption and flame emission spectrometry, TGA, DTA and DSC working principle and their instrumentation. Understand the concepts and principles of chromatographic and electroanalytical techniques applications.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 604.1]. Understand the basic principle, instrumentation, applications of molecular spectroscopy.
[CHM T 604.2]. Learn the principle and differences of atomic absorption and emission spectrometry.
[CHM T 604.3]. Learn about the working principle and instrumentation of thermal analysis.
[CHM T 604.4]. Understand and apply the concepts of chromatographic techniques and its separation.
[CHM T 604.5]. Learn the concepts of electroanalytical technique methods and its application.

B. SYLLABUS

Unit – 1: Molecular Spectroscopy

Nature of electromagnetic radiation, electromagnetic spectrum, atomic, molecular and vibrational energy levels, basic instrumentation- source of radiation, monochromator, sample cells, absorber, detector, UV-Vis detector, photomultiplier, IR detector, display and recorder, single and double beam spectrophotometer, Beer Lambert law, deviation from beers law, ultraviolet and visible spectroscopy, Fluorescence and phosphorescence spectrophotometer, Fourier transform infrared spectrometer and Raman spectrometer, instrumentation, techniques and application.

Unit – 2: Atomic Spectroscopy

Flame emission spectrometry, atomic absorption spectroscopy- principle, instrumentation, Source in AAS – Hollow cathode lamp, electrode less discharge lamp, burners, nature and property of flame, interference in AAS, difference between AAS and FES, ICP.

Unit – 3: Thermal Analysis

Types of thermal method, Thermogam, thermogravimetric analysis (TGA), differential thermal analysis(DTA), differential scanning calorimetry (DSC), schematic diagram for TGA and DTA instruments and their working principle, factors affecting thermogram like geometry of sample holder, furnace atmosphere, heating rate, particle size, packing of sample, weight of sample, analysis of metals or oxide in mixture, application of TGA and DTA.

Unit – 4: Chromatography

Principles of chromatographic separation, classification of Chromatographic Techniques: adsorption, partition, ion exchange and size exclusion chromatography, theory of chromatographic separation, distribution coefficient, retention time, sorption, theory of column efficiency and resolution, separation factor, retention factor. – working principle and application of Column chromatography, ion exchange chromatography, paper chromatography, Thin layer chromatography (TLC) & HPTLC: techniques and application. - Gas Chromatography and high performance liquid chromatography: Van Deemter equation, retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation

efficiency and resolution, instrumentation and application.

Unit – 5: Electroanalytical Techniques

Electrochemical cells, current potential relationship, mass transfer by migration, convection and diffusion, Electrogravimetry, voltam-metry, polarography, reference electrode, working electrode, auxiliary electrode, dropping mercury electrode, current potential curve, limiting current, coulometry, conductometry methods, instrumentation, techniques and application. Amperometric titration, effect of electroactive and reagent on amperometric curve and its advantage, rotating platinum electrode, biamperometric titration and its advantage, fluorimetry and phosphorimetry.

C. Reference Books:

1. Arthur I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
2. Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
3. Gary D. Christian: *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
4. C. Daniel Harris: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
5. S. M. Khopkar: *Basic Concepts of Analytical Chemistry*, New Age, International Publisher, 2009.
6. D. A. Skoog, F. J. Holler and T. A Nieman: *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore.
7. O. Mikes & R. A. Chalmes: *Laboratory Hand Book of Chromatographic & Allied Methods*, Elles Harwood Ltd. London.
8. R. V. Ditts: *Analytical Chemistry* – Methods of separation.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 604.1	Understand the basic principle, instrumentation, applications of molecular spectroscopy.	2					1	2		1		2
CHM T 604.2	Learn the principle and differences of atomic absorption and emission spectrometry.	2		3			1	2	2	1		2
CHM T 604.3	Learn about the working principle and instrumentation of thermal analysis.	2	2	2	3	1			2			1
CHM T 604.4	Understand and apply the concepts of chromatographic techniques and its separation.	1	1						2			3
CHM T 604.5	Learn the concepts of electroanalytical technique methods and its application.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 605: BASIC OF MATERIALS CHEMISTRY (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Understand the background of the crystal structures and properties. Analyzing the crystal and solid materials by using the various characterization techniques. Explore the electronic and magnetic properties and preparation methods of solids.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 605.1]. Understand the basic crystal structures and its properties.
[CHM T 605.2]. Apply the characterization techniques to know the crystal and solid materials properties.
[CHM T 605.3]. Learn about the defects and phase transitions of crystal and solid materials.
[CHM T 605.4]. Understand the electronic and magnetic properties.
[CHM T 605.5]. Learn the crystal and solid materials preparative methods.

B. SYLLABUS

Unit – 1: Chemical Crystallography

***Introduction*:** Space lattice, crystal point groups, space group (working knowledge), stereographic projections, packing in solids, crystal structures of representative systems, silicates and zeolites, cements, glasses, quasicrystals, nanostructures.

***Bonding in Solids and Crystal Energetics*:** Crystal classifications, Madelung constant and Lattice energy.

Unit – 2: Characterization Techniques for Solids

X-ray diffraction, electron microscopy (SEM, TEM, AFM), thermal techniques (TG, DTA, DSC), spectroscopic techniques (Mössbauer, IR, UV-VIS), and physical property measurement techniques (magnetic moments-VSM/SQUID, electrical resistivity – two / four probe methods and thermal conductivity, optical band gap, XPES, XAS.

Unit – 3: Electronic and Magnetic Properties Solids

Electronic Properties and Band Theory of Solids: Free electron theory of metals, Band theory of solids, Bloch theorem, Kroning-Penne model, refinement of simple band theory- *k*-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, *p*-*n* junctions.

***Magnetic Properties Solids*:** Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis. Introduction of superconductors, Meissner effects, basic concepts of BCH theory.

Unit – 4: Defects and Phase Transitions

***Defects, Nonstoichiometry and Diffusion*:** Point defects, dislocations, extended defects, clusters and

aggregates, color centers, nonstoichiometry of compounds, diffusion mechanisms, Fick's law, Kirkenall effect.

***Phase Transitions*:** Critical phenomena, variety of phase transitions (ordered-disorder, Martensite-austenite, spinoidal decompositions *etc*), liquid crystals, structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

Unit – 5: Preparative Techniques

***Reactivity of Solids*:** Decomposition and reactivity, solid state reactions, sintering process, reaction kinetics, organic solid reactions.

***Conventional Techniques*:** Powder mixing, fusion, precipitation from solution, modern need for improved synthetic routes, crystal growth and thin film techniques.

Chemical Routes: Wet-chemical (Oxidation-reduction for metal nanoparticles) methods, self assembly methods, reverse micelles route, biomimetic, sonochemical, and electrochemical approaches.

***Sol-Gel Synthesis*:** Colloids, cation hydrolysis and sol formation, gel precipitation, sol-gel process for colloids, synthesis andphysical properties of metal alkoxides, development of sol-gel process from alkoxides, derived coatings, fibers and monodispersed submicron/ nanostructured oxide powders, ormosils, sialons.
***Hydrothermal/Solvothermal Approach*:** Forced hydrolysis at elevated temperatures and pressures, hydrothermal reactions using salt solutions, metal reactants and reactions involving phase transformation.

***Precursor Technique*:** Citrate-gel process, metallo-organic precursors, metal alkoxides.

***Gas Phase Reactions*:** Gas-phase nucleation, flame hydrolyzed powders, direct - nitridation and carbothermic reduction, non-plasma gas phase reactions, plasma reactions, electron beam evaporation.

C. Reference Books:

1. A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
2. L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
3. A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
4. C. N. R. Rao and J. Gopalkrishanan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
5. R. E. Newnham, *Structure Property Relations*, Springer-Verlag, 1987

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 605.1	Understand the basic crystal structures and its properties.	2					1	2		1		2
CHM T 605.2	Apply the characterization techniques to know the crystal and solid materials properties.	2		3			1	2	2	1		2
CHM T 605.3	Learn about the defects and phase transitions of crystal and solid materials.	2	2	2	3	1			2			1
CHM T 605.4	Understand the electronic and magnetic properties.	1	1						2			3
CHM T 605.5	Learn the crystal and solid materials preparative methods.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 606: INTRODUCTION TO NANOMATERIALS AND NANOTECHNOLOGY (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learner are Able to: Learn the background principle nanotechnology and types of nanomaterials. Apply the basic characterization techniques to know the structure and properties of nanomaterials. Explore the basic background and importance behind the synthesis of nanomaterials and with applying the size dependent properties (mechanical, physical and chemical properties) and their various applications towards the world need.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 606.1]. Understand the background principle nanotechnology and types of nanomaterials.
[CHM T 606.2]. Learn characterization techniques for the structure and properties of nanomaterials.
[CHM T 606.3]. Learn the background and importance behind the synthesis of nanomaterials.
[CHM T 606.4]. Understand the concepts of size dependent properties while preparing nanomaterials.
[CHM T 606.5]. Understand the nanomaterial applications towards the world requirements.

B. SYLLABUS

Unit – 1: Nanoscience and Nanotechnology

***Introduction*:** Underlying physical principles of nanotechnology: *Nanostructured Materials: Size is Everything*. Fundamental physicochemical principles, size and dimensionality effects; quantum confinement; properties dependent on density of states; single electron charging, central importance of nanoscale morphology. Societal aspects of nanotechnology: health, environment, hype and reality.

***Type of Nanostructures*:** Definition of a nano system; one dimensional (1D), two dimensional (2D), three dimensional (3D) nanostructured materials; quantum dots; quantum wire, and core/shell structures.

Unit -2: The Basic Tools of Nanotechnology

Electron microscopy (SEM, TEM with EDX analysis) and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM); an introduction and basic principles & applications of XPS, FTIR spectrophotometers; UV-VIS principle and application for band gap measurement.

Unit – 3: Synthesis of Nanomateirals

Top down and bottom up approaches to synthesis of nanomaterils:

***Chemical Routes for Synthesis of Nanomaterials*:** Chemical precipitation and co-precipitation; sol-gel synthesis; microemulsions or reverse micelles; solvothermal synthesis; thermolysis routes, microwave heating synthesis biomimetic and electrochemical approaches; sonochemical synthesis; photochemical synthesis; synthesis in supercritical fluids.

***Physical Routes for Preparation of Nanomaterial*:** Inert gas condensation, arc discharge, RF plasma, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, spray pyrolysis, ball milling, molecular beam epitaxy, chemical vapour deposition method, Langmuir-Blodgett (LB) films, spin coating and electro deposition.

Unit – 4: Nanomateirals and Properties

Synthesis and size dependent properties (mechanical, physical and chemical properties) of carbon nanotubes (CNT); metals (Au, Ag); metal oxides (TiO_2, CeO_2, ZnO); semiconductors (Si, Ge, CdS, ZnSe); dilute magnetic semiconductor.

Unit -5: Applications of Nanomateirals

Basic ideas of nanodevices (molecular electronics and nanoelectronics, and quantum electronic devices); CNT based transistor and field emission display; biological applications; biochemical sensor; membrane based water purification, energy storage devices, catalysis and various related fields.

C. Reference Books:

1. T. Pradeep, *Nano: The Essentials*, Tata McGraw-Hill, New Delhi, 2007.
2. G. Cao, *Nanostructures and Nanomaterials – Synthesis, Properties and Applications*, Imperial College Press, London, 2004,
3. C. N. R. Rao, A. Muller and A. K. Cheetham, *The Chemistry of Nanomaterials*
4. G. L. Hornyak, J. J. Moore, H. F. Tibbals, and J. Dutta: *Fundamentals of Nanotechnology*, CRC Press, 2009

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 606.1	Understand the background principle nanotechnology and types of nanomaterials.	2					1	2		1		2
CHM T 606.2	Learn characterization techniques for the structure and properties of nanomaterials.	2		3			1	2	2	1		2
CHM T 606.3	Learn the background and importance behind the synthesis of nanomaterials.	2	2	2	3	1			2			1
CHM T 606.4	Understand the concepts of size dependent properties while preparing nanomaterials.	1	1						2			3
CHM T 606.5	Understand the nanomaterial applications towards the world requirements.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 607: POLYMERS CHEMISTRY (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basic importance of polymers and classification based on parametric way. Explore the characterization techniques to understand the chemical, thermal, physical properties. Understand the polymer processing and properties of commercial polymers.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 607.1]. Learn the importance of polymers and its classifications.
[CHM T 607.2]. Learn the thermal, physical properties polymers by using characterization techniques.
[CHM T 607.3]. Learn the characterization techniques to know the structure and chemical properties of polymer materials.
[CHM T 607.4]. Understand the concepts of polymer processing.
[CHM T 607.5]. Learn the idea behind the properties of commercial polymers.

B. SYLLABUS

Unit – 1: Introduction

Importance of polymers. Basic Concept: monomers, repeat units, degree of polymerization; linear, branched, and network polymers (block-copolymer, dendrimer etc.); classification of polymers. Polymerization: condensation, addition, radical, chain- ionic- and co-ordination-, and co-polymerization; polymerization condition and polymer reaction; polymerization in homogeneous and heterogeneous systems.

Unit– 2: Polymer Characterization Techniques

Polydispersion-average molecular weight concept; number, weight and viscosity average molecular weights. Polydiversity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group, viscosity, light scattering, osmotic, and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers. Spectroscopic methods, X-ray diffraction, microscopy studies. Thermal analysis and physical testing tensile strength, fatigue, impact, tear resistance, hardness and abrasion resistance analysis.

Unit – 3: Structure and Properties

Morphology and order in crystalline polymers – configuration of polymer chains; crystal structure of polymers; morphology of crystalline polymers; strain-induced morphology; crystallization and melting polymer structure and physical properties – crystalline melting point, T_m, melting points of homogeneous series effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g, relationship between T_m and T_g, effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Properties requirements for polymer utilization.

Unit – 4: Polymer Processing

Plastic, elastomers and fibres, compounding; processing techniques- calendaring, die casting, rotational casting, film casting, injection casting, blow moulding, extraction moulding, thermoforming, foaming, reinforcing, and fibre spinning.

Unit – 5: Properties of Commercial Polymers

Polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resins, epoxy resins and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

C. Reference Books:

1. Fred W. Billmeyer: *Textbook of Polymer Science*, Eds: 3rd, Wiley-India, New Delhi, 2012.
2. A Ravve: *Principle of Polymer Chemistry*, Eds. 3rd, Springer Science + Business Media, New York, 2012.
3. J. M. G. Cowie: *Physics and Chemistry of Polymers*, Blackie Academic and Professional.
4. H. R. Alcock and F. W. Iamtee: *Contemporary Polymer Chemistry*, Prentice Hall.
5. V. R. Govarikar, N. V. Viswanathan, and J. sreedhar: *Polymer Science*, Wieley-Eastern.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 607.1	Learn the importance of polymers and its classifications.	2					1	2		1		2
CHM T 607.2	Learn the thermal, physical properties polymers by using characterization techniques.	2		3			1	2	2	1		2
CHM T 607.3	Learn the characterization techniques to know the structure and chemical properties of polymer materials.	2	2	2	3	1			2			1
CHM T 607.4	Understand the concepts of polymer processing.	1	1						2			3
CHM T 607.5	Learn the idea behind the properties of commercial polymers.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 608: BIOORGANIC AND DRUG CHEMISTRY (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Get the idea on bioorganic chemistry and inter disciplinary area between chemical and biology in daily life and general structure & classification of carbohydrates, proteins, lipids, and nucleic acids. Explore the similarities between biochemical and organic reactions, and basics on drug chemistry and drug action. Get the idea on structure and importance of pharmaceutical compounds in daily life.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 608.1]. Learn the basics in bioorganic chemistry and relations between chemical and biology.
[CHM T 608.2]. Learn the basic introduction of structure & classification of carbohydrates, proteins, lipids, and nucleic acids.
[CHM T 608.3]. Learn about the similarities between biochemical and organic reactions.
[CHM T 608.4]. Understand the basics on drug chemistry and drug action.
[CHM T 608.5]. Understand the importance of pharmaceutical compounds in daily life.

B. SYLLABUS

Unit – 1: Overview of Bioorganic Chemistry

***Introduction*:** Definition of bioorganic chemistry, Border line of bioorganic chemistry and inter disciplinary area between chemical and biology, Weak interaction in organic and biological world, Molecular Recognition.

***Chemistry of the Living Cell*:** The structure of prokaryotic and Eukaryotic cells, Composition of living cells:

Unit – 2: Carbohydrates, Proteins, Lipids, and Nucleic Acids

***Carbohydrates*:** Introduction, Reactions of Monosaccharides, Interconversions, Ring structure of aldoses and ketoses, Confirmation of Monosaccharides, Disaccharides: Structure, synthesis and properties.

***Proteins*:** General structure & classification of amino acids, Abbreviation of amino acids, Essential and non essential amino acids, Synthesis of amino acids, Isoelectric point, Acid and base properties of amino acids. Protein: Naturally occurring peptides, Modern methods of peptide synthesis with protection and deprotection, Determination of sequences and basic units of a poly peptides or proteins, C- & N-terminus detection by chemical methods, Primary, secondary, tertiary and quaternary structures of proteins, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases etc.

***Lipids*:** Lipid structure- acylglycerols, phosphoglycerides and sphingolipids, Biological importance of fatty acids and lipids, Bio- and chemical Synthesis of lipids.
***Nucleic Acids*:** Definition, structure and properties, base pairing, double helices, Genetic information storage, transmission and gene expression, Nucleotides and Nucleosides: Similarities and differentiation, Structure of DNA & RNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis.

Unit – 3: Analogy Between Biochemical and Organic reactions

Introduction to metabolism (catabolism, anabolism). ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD^+, FAD. Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle. Overview of catabolic pathways of fat and protein. Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types.

Unit – 4: Overview of Drug Chemistry and Basics of Drug Action

Definition, classification and nomenclature of drugs, Preliminary idea of drug action: Interaction (Weak interaction in drug molecules, Chirality and drug action), Receptorology (Drug-receptor interactions, Enzyme kinetics in drug action, Enzyme inhibitors (Drug action through enzyme inhibition), Nucleic acids as targets for drug actions, NA-Alkylation, NA-strand breaking and their importance in drug action, Drug metabolism, drug deactivation and elimination.

Unit – 5: Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

Reference Books:

1. L. Stryer: *Biochemistry*, 4th Edition W. H. Freeman and Co. 1995.
2. S. Zubay: *Biochemistry*, Addison-Wesely 1983.
3. J. Mann; R.S. Davidson: *Natural Products: Chemistry and Biological Significance*
4. H. Dugas: *Bioorganic Chemistry Frontiers Vol. 2*, ed. Springer-Verlag, 1990.
5. E. E. Tamlen: *Bioorganic Chemistry*, Academic Press, 1977.
6. M. Bodansky: *Peptide Chemistry: A Practical Textbook*, Springer-Verlag 1988.
7. *Bioorganic Chemistry: A chemical approch to enzyme action*, Springer-Verlag 1989.
8. W. Saenger: *Principles of Nucleic acid structures*, Springer-Verlag 1984.
9. G. R. Chatwal: *Medicinal Chemistry*
10. A. Kar: *Medicinal Chemistry*, Wiley, 2000.
11. D. Lednicer: *Strategies for Organic Drug Synthesis and Design*, John Wiley 1998.
12. G. R. Chatwal: *Synthetic Drugs*, Himalaya, New Delhi 1995.
13. S. Hanessian, *Total synthesis of Natural product: The chiral approach Vol.III* Pergamon Press 1983.
14. W. D. Foye, T. L. Lemke, and D. A. Williams: *Principles of Medicinal Chemistry (*4th Edition)
15. R. B. Siwerman: *Organic Chemistry of Drug Action and Design* (Academic press, 1993).

C. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 608.1	Learn the basics in bioorganic chemistry and relations between chemical and biology.	2					1	2		1		2
CHM T 608.2	Learn the basic introduction of structure & classification of carbohydrates, proteins, lipids, and nucleic acids.	2		3			1	2	2	1		2
CHM T 608.3	Learn about the similarities between biochemical and organic reactions.	2	2	2	3	1			2			1
CHM T 608.4	Understand the basics on drug chemistry and drug action.	1	1						2			3
CHM T 608.5	Understand the importance of pharmaceutical compounds in daily life.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 609: ADVANCED HETEROCYCLIC CHEMISTRY (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Know the basic idea on aromatic and non-aromatic heterocyclic compounds and about the strains, interactions and conformational aspects of non-aromatic heterocycles. Explore the basics of five and six membered heterocyclics with one and two hetero atom and larger ring heterocyclics.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 609.1]. Understand the basics of aromatic and non-aromatic heterocyclic compounds.

[CHM T 609.2]. Learn about the strains, interactions and conformational aspects of non-aromatic heterocycles.

[CHM T 609.3]. Learn the basics on five and six membered heterocyclics with one hetero atom.

[CHM T 609.4]. Learn the basic idea on synthesis and reactions of five and six membered heterocyclics with one hetero atoms.

[CHM T 609.5]. Learn the basics of larger ring heterocyclics and their synthesis, structure, stability and reactivity.

B. SYLLABUS

Unit – 1: Introduction

Definition of heteroatom, Aromatic and non-aromatic heterocyclic compounds, Classification and nomenclature of heterocyclic compounds, important reactions with heterocyclic compounds i.e. oxidation, reduction and tertiary effect of Nitrogen in heterocyclic compound.

Unit – 2: Non-Aromatic Heterocycles

Different types of strains, interactions and conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of the following ring systems: Aziridines, Oxiranes, Thiiranes, Oxaziridines, Azetidines, Oxetanes and Thietanes.

Unit – 3: Five and Six Membered Heterocyclics with One Hetero Atom

Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions [Advanced synthetic methods are applied].

Unit – 4: Five and Six Membered Heterocyclics with Two Hetero Atoms

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

Unit – 5: Larger Ring and Other Heterocycles

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Benzoazepines, Benzooxepines, Benzothiepines, Azocines and Azonines.

Reference Books:

1. T. Gilchrist: *Heterocyclic Chemistry*
2. R. M. Acheson: *An Introduction to the Chemistry of Heterocyclic Compounds*
3. J. A. Joule & K. Mills: *Heterocyclic Chemistry*
4. A. Paquette: *Principles of Modern Heterocyclic Chemistry*
5. J, A. Joule & Smith: *Heterocyclic Chemistry*
6. A .R. Katritzky: *Handbook of Heterocyclic Chemistry*

C. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 609.1	Understand the basics of aromatic and non-aromatic heterocyclic compounds.	2					1	2		1		2
CHM T 609.2	Learn about the strains, interactions and conformational aspects of non-aromatic heterocycles.	2		3			1	2	2	1		2
CHM T 609.3	Learn the basics on five and six membered heterocyclics with one hetero atom.	2	2	2	3	1			2			1
CHM T 609.4	Learn the basic idea on synthesis and reactions of five and six membered heterocyclics with one hetero atoms.	1	1						2			3
CHM T 609.5	Learn the basics of larger ring heterocyclics and their synthesis, structure, stability and reactivity.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 610: CHEMISTRY OF NATURAL PRODUCTS (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basic properties, structure and biological role of alkaloids, steroid, terpenes and vitamins.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 610.1]. Learn the classification of alkaloids on the basis of amino acid origin and present core structure.

[CHM T 610.2]. Understand the structure and biological role of nicotine, cocaine, quinine, and reserpine.

[CHM T 610.3]. Learn the introduction, nomenclature, configuration and properties of steroids.

[CHM T 610.4]. Learn the introduction, classification and structure and properties of terpenes.

[CHM T 610.5]. Learn the introduction, structure elucidation and biological role of vitamins.

B. SYLLABUS

Unit – I: Alkaloid – I

Occurrence and isolation, biological role of alkaloids, General properties, nomenclature and classification of alkaloids on the basis of amino acid origin and present core structure. Isolation, properties and structural elucidation of quinine, Morphine (structure, synthesis, molecular rearrangement, stereochemistry and biogenesis).

Unit – II: Alkaloid – II

Structure and biological role of nicotine, cocaine, quinine, reserpine, vincristine, morphine, caffeine, papavarine, hyocimine. Strychnine and lysergic acid.

Unit – III: Steroid

Introduction, nomenclature of steroids, absolute configuration of steroid. Occurrence, isolation, structute elucidation and chemical properties of Cholesterol.

Unit – IV: Terpenes

Secondary metabolites: Definition and examples; terpenes – isoprene rule; mono terpenes: structure of geraneol, limonene, alpha-pinene and camphor; sesquiterpenes: longfolene;

diterpenes: abietic acid, taxol. Structure determination of Citral and Camphor.

Unit – V: Vitamins

Introduction, chemical properties, structure elucidation of Vitamin A, Vitamin B, Ascorbic Acid and Vitamin D. Vitamin A and its role in vision. Biological role of Vitamin D, Ascorbic Acid, Vitamin A.

C. Reference Books:

1. I. L. Finar: *Organic Chemistry Vol. II*, 5th Edition
2. S. V. Bhat, B. A. Nagaramgagi, M. Srikumar: *Chemistry of Natural Products*, Alpa Science International Ltd, 2005 by
3. O. P. Agarwal: *Chemistry of Natural Products, Vol I & Vol II*, Goel publishing House, 1989
4. J. R. Hanson: *Natural Products: The Secondary Metabolites*, Wiley-Vch, 1st Ed.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 610.1	Learn the classification of alkaloids on the basis of amino acid origin and present core structure.	2					1	2		1		2
CHM T 610.2	Understand the structure and biological role of nicotine, cocaine, quinine, and reserpine.	2		3			1	2	2	1		2
CHM T 610.3	Learn the introduction, nomenclature, configuration and properties of steroids.	2	2	2	3	1			2			1
CHM T 610.4	Learn the introduction, classification and structure and properties of terpenes.	1	1						2			3
CHM T 610.5	Learn the introduction, structure elucidation and biological role of vitamins.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 611: SOLID STATE CHEMISTRY (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn about the basics of crystalline and amorphous materials and solids symmetry in crystals, basic crystal systems, space groups. To learn the structure and properties of advance materials.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 611.1]. Understand the basics of crystalline and amorphous materials and crystal structure.
[CHM T 611.2]. Learn about symmetry operation and symmetry elements crystalline materials.
[CHM T 611.3]. Learn about point groups crystalline materials.
[CHM T 611.4]. Understand the structure and properties of inorganic hybrid materials.
[CHM T 611.5]. Understand the structure and properties of organic-inorganic hybrid materials.

B. SYLLABUS

Unit – 1: Crystal Structure

Crystalline and amorphous solids; symmetry in crystals, basic crystal systems,space lattice and unit cell, Bravais lattice,miller indices, closed packed structure- hcp and ccp, packing efficiency, limiting radius ratio and shape of ionic crystal, description of solids; structure types Rock salt (NaCl), Zinc blende (ZnS),antifluorite(Na_2O), Rutile (TiO_2), Wurzite (ZnS), $CdCl_2$, nickel arsenide, CsCl, CdI2, Cs_2O, perovskite ABO_3, K_2NiF_4, spinels.

Unit – 2: Point Groups

Symmetry operation and symmetry elements, Plane of symmetry, inversion centre, proper and improper axis of rotation, Product of symmetry operation, Relation among symmetry elements and symmetry operation, classification of symmetry, symmetry elements in octahedral and tetrahedral molecules, symmetry point group, representation of symmetry operation by matrices, reducible and irreducible representation, Character tables.

Unit – 3: Space Groups

Thirty two point groups, Representation of point groups and selected examples like 222, mm2, mmm, 32 centrosymmetric and noncentrosymmetric point groups, space group: Triclinic P1, monoclinic C2, monoclinic C2/m, orthorhombic $P222_1$ orthorhombic F222, Tetragonal 14_1 , space group and crystal structure of $SrTiO_3$ and rutile structure of TiO_2.

Unit – 4: Structure and Properties of Advance Materials – I

Superconductors – (Ba,K)BiO_3, Cuprates, LnFeAsO, MgB_2, CaC_6
CMR materials – $La_{(1-x)}Sr_xMnO_3$
Ferroic compounds – $BaTiO_3$, $PbTiO_3$, $Bi_4Ti_3O_{12}$, $SrRuO_3$
Peizoelectric materials- PZT,
Photoluminescent materials – Lanthanide compounds
Porous materials – zeolites, AlPO, MeAlPO, SAPO.

Unit – 5: Structure and Properties of Advance Materials – II

Organic-inorganic hybrid materials – MOF compounds
Ionic Conductors – NASICON, AgI, $NaAl_{11}O_{17}$
Thermoelectric materials – $NaxCoO_2$, $AgSbTe_2$, $CoSb_3$, $Y_{14}MnSb_{11}$

Compounds for intercalation and redox reactions – $LiCoO_2$, $LiVS_2$, NASICON, Chevrel phases

C. Reference Books:

1. C. N. R. Rao and J. Gopalakrishnan: *New Direction in Solid State Chemistry*, Cambridge University Press, 1997.
2. A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
3. L. Smart and E. Moore: *Solid State Chemistry*, Chapman and Hall, 1992.

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 611.1	Understand the basics of crystalline and amorphous materials and crystal structure.	2					1	2		1		2
CHM T 611.2	Learn about symmetry operation and symmetry elements crystalline materials.	2		3			1	2	2	1		2
CHM T 611.3	Learn about point groups crystalline materials.	2	2	2	3	1			2			1
CHM T 611.4	Understand the structure and properties of inorganic hybrid materials..	1	1						2			3
CHM T 611.5	Understand the structure and properties of organic-inorganic hybrid materials.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

PAPER CODE: CHM T 612: ADVANCED SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE)

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basics of metal mediated C-C and C-X coupling, oxidation and reduction and also protection-deprotection of functional groups C-C and C-X coupling reactions and other important organic reactions.

A. Course Outcomes: At the end of the course, students will be able to

[CHM T 612.1]. Understand the basics of metal mediated C-C and C-X coupling reactions.
[CHM T 612.2]. Learn the P, S, Si, and B containing compounds-preparations and organic reactions.
[CHM T 612.3]. Learn about oxidation and reduction reaction of organic reactions.
[CHM T 612.4]. Learn the protection-deprotection of functional groups C-C and C-X coupling reactions.
[CHM T 612.5]. Understand the stereoselective organic reactions. And green chemistry.

B. SYLLABUS

Unit – 1: Metal Mediated C-C and C-X Coupling Reactions

Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia Lythgoe olefination and Peterson's stereoselective olefination. Olefin metathesis by I^{st} and II^{nd} generation catalysts: Reaction mechanism and application in the synthesis of heterocycles.
Phosphorous Sulfur, Silicon and Boron containing compounds-preparations and their uses in organic reactions.

Unit– 2: Reagents of Phosphorous, Sulfur, Silicon and Boron (12 Hours)

Phosphorous Sulfur, Silicon and Boron containing compounds-preparations and their uses in organic reactions.

Unit – 3: Oxidation and Reduction

***Oxidation*:** Oxidation of hydrocarbons (alkanes, aromatic hydrocarbons, alkenes), Oxidation of alcohols (Chromium reagents, Manganese reagents, Other metal and non-metal based oxidants), Oxidation of ketones (α, β-unsaturated ketones, α-hydroxy ketones, Baeyer-Villiger oxidation of ketone)
***Reduction*:** Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents (Derivatives of lithium aluminium hydride and sodiumborohydride, mixed lithium aluminium hydride-aluminium chloride reagent, DIBAL-H, $NaBH_3CN$, sodium triacetoxyborohydride, Borane and derivatives, other methods of reductions).

Unit – 4: Disconnection Approach, Umpolung Chemistry and Protection-Deprotection of Functional groups

Basic principles and terminology-Target molecule, FGI, Disconnection, Synthon, Reagent and Retro-synthetic approach. **One group C-C and C-X disconnection**: (disconnection of alcohols, alkenes, and carbonyl compounds). **Two group C-C & C-X disconnections**: 1,3 and 1,5 difunctionalised compounds, α, β, unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels- Alder reaction, connection in retro synthesis. Umpolung in organic synthesis.

Protection and deprotection for functional groups as hydroxyl, amino, carboxylic and carbonyl.

Unit – 5: Some Important Organic Reactions

Selective Stereoselective Organic Reactions with Alkenes: Sharpless Asymmetric Epoxidation, Asymmetric Aziridination, Dihydroxylation, Amino-hydroxylation Reactions, Oxidative cleavages of alkenes.

Green Chemistry, Supramolecular chemistry (Crown ether, Cyclodextrin and Clalixerins) and multicomponent reactions (Ugi, Passerini, Biginelli, Hantzsch reactions).

***Chemistry of Aliphatic and Aromatic Heterocyclic Compounds*:** Epoxide, Aziridine, Azitidine, Oxetane, Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions.

C. References Books:

1. B. F. G. Johnson: *Transition Metal Cluster*, Wiley, 1980.
2. R. H. Crabtree: *The Organometallic Chemistry of the Transition Metals*, Wiley-Interscience, 2005.
3. G. Wikinson, F. G. A. Stone, and E. Abel: *Comprehensive Organometallic Chemistry*, Peramon, 1980.
4. I. Fleming: *Frontier Orbitals and Organic Chemical Reactions,* Wiley, 1976.
5. B. B. Woodward and Hoffman: *Conservation of Orbital Symmetry*, Verlag Chemie Academic Press, 1971.
6. S. Warren: *Organic Synthesis: The Disconnection Approach,* John Wiley & Sons (Asia) Pte. Ltd., 2007
7. W. Carruthers and I. Coldham: *Modern Methods of Organic Synthesis*, Fourth Ed. Cambridge University Press.
8. T. L. Gilchrist: *Heterocyclic Chemistry*, Pearson Education, 3rd Ed.2007

D. Course Articulation Matrix: (Mapping of COs with POs)

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHM T 612.1	Understand the basics of metal mediated C-C and C-X coupling reactions.	2					1	2		1		2
CHM T 612.2	**].** Learn the P, S, Si, and B containing compounds-preparations and organic reactions.	2		3			1	2	2	1		2
CHM T 612.3	Learn about oxidation and reduction reaction of organic reactions.	2	2	2	3	1			2			1
CHM T 612.4	Learn the protection-deprotection of functional groups C-C and C-X coupling reactions..	1	1						2			3
CHM T 612.5	Understand the stereoselective organic reactions. And green chemistry.	1		3	1			1	1			3

1- Low Correlation; 2- Moderate Correlation; 3- Substantial Correlation

Indira Gandhi National Tribal University, Amarkantak (MP)

Ph. D. Course Work Syllabus of Chemistry

Core Paper	Course code	Title of the course	Credits	Marks
	PCC- 1101	Research Methodology	4	100
	PCC- 1102	Computer Applications and Data Analysis	4	100
	PCC- 1103	Research & Publication Ethics	2	50
Discipline Specific Elective Paper (Opted any one of the DET Course)				
DSET	CHE DET 1104-1115	Discipline Specific Elective Theory (DET) paper opted from any one of the following courses	4	100
	CHE DEP 1116	Chemistry Practical	2	50
		Total	16	400

Discipline Specific Elective Theory

*

Course Code	Title of Paper	Credit	Marks
CHE DET 1104	Advanced Analytical Chemistry	04	100
CHE DET 1105	Advanced Organometallic Chemistry	04	100
CHE DET 1106	Modern Physical Methods in Chemistry Research	04	100
CHE DET 1107	Advanced Materials Chemistry	04	100
CHE DET 1108	Principles of X-ray Diffraction and Electron Microscope	04	100
CHE DET 1109	Advanced Electro Chemistry	04	100
CHE DET 1110	Polymers Chemistry	04	100
CHE DET 1111	Chemistry of Natural Products	04	100
CHE DET 1112	Advanced Synthetic Organic Chemistry	04	100
CHE DET 1113	Advanced Heterocyclic Chemistry	04	100
CHE DET 1114	Bioorganic and Drug Chemistry	04	100
CHE DET 1115	Molecular Recognition & Supra Molecular Chemistry	04	100

Notes:

- **Research scholars those who studied above mentioned courses in their PG Programme they must opt different course.**
- **All the elective papers will be offered as suggested by the concern DRC.**

PCC – 1101

RESEARCH METHODOLOGY

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: An Overview of Research Methodology

Research concept, steps involved, identification, selection and formulation of research problem, justification, hypothesis; literature collection- textual and digital resources (internet)

Unit – II: Research Design, Data Collection &Interpretation

Research design; sampling techniques, collection and documentation, presentation, analysis and interpretation of data

Unit – III: Scientific Writing and Formulation of Scientific Communication

Forms of scientific writing- Article, notes, reports, review article, monographs, dissertations, popular science articles, bibliographies

Outline preparation, drafting title, sub titles, tables, illustrations; Formatting tables- title, body footnotes; figures & graphs- structure, title and legends, Impact factor, citation indices, plagiarism

Unit – IV: Good Laboratory Practices and Safety Measures

Recording and storage/ retention of recorded materials, Maintenance of equipments, Storage and disposal of hazardous materials (chemical and biological), Management and user responsibilities in proper utilization of the facilities, Handling of radiation, Bio-hazardous and other toxic experimental materials

Suggested Readings:

1. Research Methodology - Methods & Techniques, CR Kothri CR (1990), VishvaPrakashan, New Delhi.
2. Research Methodology & Statistical Techniques, S Gupta (1999) Deep & Deep Publications, New Delhi.
3. Research Methodology for Biological Sciences, N Gurumani (2007), MJP Publishers, Chennai.
4. Principles and techniques of Biochemistry and Molecular Biology, 7th Ed: K. Wilson, J. Walker, Cambridge Univ. Press. UK
5. An Introduction to Practical Biochemistry, 3rd Ed : D. T. Plummer, Tata-McGraw Hill
6. Modern Experimental Biochemistry and Molecular Biology 2nd Ed: R. Boyer
7. Benjamin/Cumin
8. Physical Biochemistry, 2nd Ed: D.M. Freifelder, Freeman Press.
9. Analytical Biochemistry, 3rd Ed. D. Holme, J. Peck, Tata McGraw Hill.
10. Experimental Biochemistry, 3rd Ed: R. L. Switzer, L.F. Garrity, Freeman Press

PCC – 1102

COMPUTER APPLICATIONS AND DATA ANALYSIS

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Computers, operating systems and useful software

MS-windows and Linux; utility of Latex, MS-Office and LibreOffice for presentation and communication of research. Spreadsheets: Excel and SPSS; importing data files to statistical software; Using SPSS / R: creating variables, data entry; Descriptive data analysis: Frequencies cross tabulations and layers; Graphical tools available with Excel / R / Origin.

Unit – II: World Wide Web and Research

Electronic mail; E-Journals and E-library; using research specific search engines like Google Scholar; Journal indexing databases: SCOPUS and Web of Science; Useful research networking platforms: Academia, Linkedin and Research Gate; Showcasing research profiles at platforms like ORCID, Publons, Google Scholar, Loop and Microsoft Academic; Working with reference management tools like Endnote, Zotero, Mendeley etc; Shodhganga repository and archiving of research papers. Selecting appropriate journals for publication.

Unit – III: Analyses of experimental data (Data Analyses with Statistical Software)

Terminology in experimental designs, principles of design, completely randomized design, randomized

block designs, Latin square design; Analysis of experimental data; Data analysis based on ANOVA and ANCOVA models.

Unit – IV: Analyses of sample survey data (Data Analyses with Statistical Software)

Basic principles of sample surveys, different steps in a sample survey; Techniques of random sampling: simple random sampling, stratified random sampling and systematic sampling; Purposive sampling and Quota sampling.

Suggested Readings:

1. Goon A.M., Gupta M.K. and Dasgupta B. (2002): Fundamentals of Statistics, Vol. II, 8th Edn. The World Press, Kolkata.
2. Introduction to Biostatistics, L Forthofer (1995), Academic Press, New York.
3. Biostatistical Analysis, JH Zar (2006), Prentice-Hall.
4. Research Design: Qualitative, Quantitative & Mixed Method Approaches, John W. Creswell (2009), Sage Publication, USA.
5. Experimental Design & Data Analysis for Biologists. PQ Gerry & JK Michael (2002), Cambridge University Press.
6. Choosing & Using Statistics: A Biologists Guide, D Calvin (2003), Blackwell Publisher.

PCC – 1103

RESEARCH & PUBLICATION ETHICS

(Credits- 02; Contact hours - 30h; Maximum marks - 50)

Unit – I: Philosophy & Ethics (3h)

Introduction to philosophy: definition, nature and scope, concept, branches.

Ethics: definition, moral philosophy, nature of moral judgements and reactions.

Unit – II: Scientific Conduct (5h)

Ethics with respect to science and research; intellectual honesty and research integrity; scientific misconducts – falsification, fabrication and plagiarism (FFP); redundant publications – duplicate and overlapping publications, salami slicing; selective reporting and misrepresentation of data.

Unit – III: Publication Ethics (7h)

Publication ethics – definition, introduction and importance, best practices/standard setting initiatives and guidelines – COPE, WAME; conflicts of interest; publication misconduct – definition, concept, problems that led to unethical behavior vice-versa, types; violation of publication ethics -, authorship and contributionship; Identification of publication misconducts, complaints and appeals; predatory publishers and journals.

Practices –

Open Access Publishing (4h)

Open access publications and initiatives; SHERPARoMEO online resource to check publishers copyright & self-archiving policies; software tool to identify predatory publications developed by SPPU; journal finder/journal suggestion tools viz., JANE; Elsevier Journal Finder; Springer Journal Suggester etc.

Publication Misconduct (4h)

Group discussions – subject specific ethical issues, FFp, authorship; conflicts of interest; complaints and appeals - examples from India and abroad (**2h**).

Software tools – use of plagiarism tools like Turnitin, Urkund and other open source software tools (**2h**).

Databases and Research Matrices (7h)

Databases – Indexing databases; citation databases – Web of Science, SCOPUS etc**(4h).**

Research matrices – Impact factors of journals as per Journal Citation Reports, SNIP, SJR, IPP, cite score;

Matrices – h-index, g-index, i10 index, altmetrics **(3h).**

Suggested Readings:

1. Bird, A. (2006). Philosophy of Science. Routledge.
2. MacIntyre, Alasdair (1967) A Short History of Ethics. London.
3. P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978- 9387480865
4. National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition. National Academics Press.
5. Resnik, D. B. (2011). What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm
6. Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179-17. https://doi.org/10.1038/489179a
7. Indian National Science Academy (INSA), Ethics in Science Education, Research and Govermance(2019), ISBN:978-81-939482-1-7.

http://www.insaindia.res.in/pdf/EthicsBook.pdf

Discipline Specific Elective Theory* (DET) (opt any one)

CHE DET 1104: Advanced Analytical Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Advanced Molecular Spectroscopy & Data Interpretation

Nature of electromagnetic radiation, electromagnetic spectrum, atomic, molecular and vibrational energy levels, basic instrumentation- source of radiation, monochromator, sample cells, absorber, detector, UV-Vis detector, photomultiplier, IR detector, display and recorder, single and double beam spectrophotometer, Beer Lambert law, deviation from beers law, ultraviolet and visible spectroscopy, Fluorescence and phosphorescence spectrophotometer, Fourier transform infrared spectrometer and Raman spectrometer, instrumentation, techniques and application.

Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of significance, rejection of a result.

Unit – II: Thermal Analysis & Atomic Spectroscopy

Types of thermal method, Thermogam, thermogravimetric analysis(TGA), differential thermal analysis(DTA), differential scanning calorimetry (DSC), schematic diagram for TGA and DTA

instruments and their working principle, factors affecting thermogram like geometry of sample holder, furnace atmosphere, heating rate, particle size, packing of sample, weight of sample, analysis of metals or oxide in mixture, application of TGA and DTA.
Flame emission spectrometry, atomic absorption spectroscopy- principle, instrumentation, Source in AAS – Hollow cathode lamp, electrode less discharge lamp, burners, nature and property of flame, interference in AAS, difference between AAS and FES, ICP.

Unit – III: Purification Technique

Chromatography

Principles of chromatographic separation, classification of Chromatographic Techniques: adsorption, partition, ion exchange and size exclusion chromatography, theory of chromatographic separation, distribution coefficient, retention time, sorption, theory of column efficiency and resolution, separation factor, retention factor. – working principle and application of Column chromatography, ion exchange chromatography, paper chromatography, Thin layer chromatography (TLC) & HPTLC: techniques and application. - Gas Chromatography and high performance liquid chromatography: Van Deemter equation, retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Solvent extraction

Theory, efficiency, percentage extraction, separation factor, complexing agent in solvent extraction, selection of solvent.

Ion- exchange

Principle, quality of resins, ion exchange equilibrium, ion exchange capacity process, deionization of water.

Unit – IV: Electrochemical analyses

Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, limiting current, current – voltage relationship during electrolysis. Electrogravimetry, voltam-metry, polarography, reference electrode, working electrode, auxiliary electrode, dropping mercury electrode, Principles and applications of Voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogavimetry.

Unit – V: Gravimetric Analysis & Quantitative Estimation

Advantage of gravimetric analysis, requirement, preparation of solution, precipitating reagent, condition for analytical precipitation, saturation and super-saturation, von Weimarn equation, co-precipitation, digestion, Ostwald ripening, aggregation and agglomeration, colloidal solution, adsorption, primary and secondary layer adsorption, peptization, impurity, inclusion and occlusion, surface adsorption, post precipitation, filtration, washing and weighing precipitate mathematical calculation on gravimetry.
Basic principle of acid base indicator, Redox titration- titration of Mohr salt against $KMnO_4$, complexometric titration- EDTA titration, Eriochrome black T indicator, complexometric titration curve, direct and back titration, masking and demasking of cations, precaution in volumetric titration, titration & Justification of Fe^{3+} and Mn^{2+} salt both in complexometry and Spectrophotometry analysis.

Reference Books:

- D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995
- G. D.Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.
- I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Gary D. Christian: *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
- C. Daniel Harris: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.
- S. M. Khopkar: *Basic Concepts of Analytical Chemistry*, New Age, International Publisher, 2009.
- D. A. Skoog, F. J. Holler and T. A Nieman: *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore.

CHE DET 1105: Advanced Organometallic Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Organometallics

Compounds with metal carbon σ and multiple bond: Haptacity complexes of Metal-alkyl, -allyl, aryl, -carbene (Fischer and Schrock type), -carbonyl, -carbines and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity and decomposition pathway, Reactions in organometallic compounds. Stucture and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_2H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, techniques of study.

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Unit – II: Catalysis

Catalysis of organometallic compounds: Ni, Pt, Pd, Co, Zn, Cd catalyst used in various organic transformation reactions.

Nanocatalysts: Used in Different photocatalytic reaction, Oxidative addition, reduction reaction, Knoevenagel Condensation Reaction, Suzuki Coupling reaction, Unsaturation reaction etc.

Unit – III: Synthesis & Characterization

Synthesis: Synthesis of different transition/novel metal based organometallic compounds by using various techniques like diffusion method, slow evaporation method, hydrothermal method, distillation, Microwave synthesis etc.

Characterization: The single crystal was characterized by Single X-ray crystallography, FTIR

Unit – IV: Recent Developments in Organometallics Chemistry Research

Construction, structure and property of compounds with specific topology in Organometallic Chemistry: Capsules, boxes, containers, prisms or clusters, tubes, catenanes, rotaxanes, incorporation of metal atoms through metal-ligand coordination interactions, Various organic ligands containing carboxy, imidazole or pyridine groups, which can coordinate with metal atoms, have been used to generate the desired compounds (V, Cr, Mn, Fe, Co, Ni, Cu). Particularly, flexible ligands with central aromatic core and imidazol-1-ylmethyl pendant arms, e.g. 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene and its analogues, Interesting properties: Molecular recognition, ion inclusion and exchange of these compounds, especially of the cage-like compounds, are described.

Unit – V: Inorganic Cages and Clusters

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds- Lipscomb's topological models, Wade`s rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

Reference Books:

- J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4th Pearson, New Delhi, 2006.
- F. A Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann: *Advanced Inorganic Chemistry*, Eds: 6th, Wiley-India, New Delhi, 2010.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
- Robert Crabtree: *The Organometallic Chemistry of the Transition Metals*, 3rd Edition, Wiley.
- Collman, Hegedus, Norton and Finke: *The Principles and Applications of Transition Metal Chemistry*, 2nd Eds, University Science Books.
- Christoph Elschenbroich: *Organometallics*, 3rd Edition,
- Wei-Yin Sun, *New Developments in Organometallics Chemistry***,** Wiley

CHE DET 1106: Modern Physical Methods in Chemistry Research

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: General Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarization, and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment selection rules, intensity of spectral line. Born-Oppenheimer approximation, rotational, vibrational, and electronic energy levels. Fourier Transform Spectroscopy.

Unit – II: Rotational and Vibrational Spectroscopy

Review of Microwave, Infrared Spectroscopy, FTIR, and Raman Spectroscopy

Unit – III: Electronic Spectroscopy and Magnetic Resonance Spectroscopy

Electronic Spectroscopy: Atomic Spectroscopy Molecular Spectroscopy and Photoelectron Spectroscopy
Magnetic Resonance Spectroscopy: Nuclear Magnetic Resonance Spectroscopy; Electron Spin Resonance Spectroscopy; Nuclear Quadrupole Resonance Spectroscopy

Unit – IV: X-ray Diffraction and Mossbauer Spectroscopy

X-ray Diffraction: Bragg condition, miller indices, Laue method, Bragg Method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absence in diffraction pattern. Structure of simple lattice and X-ray intensity, structure factor and its relation to intensity and electron density phase problem. Description of the procedure of an X-ray structure analysis.
***Mössbauer Spectroscopy*:** Basic principles, spectral parameters and spectrum display. Application of technique to the studies

Unit – V: Microscopy

Electron microscopy (SEM, TEM with EDX analysis). A brief historical overview of atomic force microscopy (AFM).

Reference Books:

- C. N. Banwell and E. M. McCash: *Fundamentals of Molecular Spectroscopy*, Ed. 4th, Tata McGraw-Hill, 1994.
- B. D. Cullity: *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, 1959.

- D. B. Williams and C. B. Carter: *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, 1996.

CHE DET 1107: Advanced Materials Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Chemical Crystallography

***Introduction*:** Space lattice, crystal point groups, space group (working knowledge), stereographic projections, packing in solids, crystal structures of representative systems, silicates and zeolites, cements, glasses, quasicrystals, nanostructures.

***Bonding in Solids and Crystal Energetics*:** Crystal classifications, Madelung constant and Lattice energy.

Unit – II: Characterization Techniques for Solids

X-ray diffraction, electron microscopy (SEM, TEM, AFM), thermal techniques (TG, DTA, DSC), spectroscopic techniques (Mössbauer, IR, UV-VIS), and physical property measurement techniques (magnetic moments-VSM/SQUID, electrical resistivity – two / four probe methods and thermal conductivity, optical band gap, XPES, XAS.

Unit – III: Electronic and Magnetic Properties Solids

Electronic Properties and Band Theory of Solids: Free electron theory of metals, Band theory of solids, Bloch theorem, Kroning-Penne model, refinement of simple band theory- *k*-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, *p*-*n* junctions.

***Magnetic Properties Solids*:** Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis. Introduction of superconductors, Meissner effects, basic concepts of BCH theory.

Unit – IV: Defects and Phase Transitions

***Defects, Nonstoichiometry and Diffusion*:** Point defects, dislocations, extended defects, clusters and aggregates, color centers, nonstoichiometry of compounds, diffusion mechanisms, Fick's law, Kirkenall effect.

***Phase Transitions*:** Critical phenomena, variety of phase transitions (ordered-disorder, Martensite-austenite, spinoidal decompositions *etc*), liquid crystals, structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

Unit – V: Preparative Techniques

***Solid State /Ball Milling*:** Decomposition and reactivity, solid state reactions, sintering process, reaction kinetics, organic solid reactions. Powder mixing, fusion, precipitation from solution, modern need for improved synthetic routes, crystal growth and thin film techniques.

Chemical Routes: Wet-chemical (Oxidation-reduction for metal nanoparticles) methods, self assembly methods, reverse micelles route, biomimetic, sonochemical, and electrochemical approaches.

***Sol-Gel Synthesis*:** Colloids, cation hydrolysis and sol formation, gel precipitation, sol-gel process for colloids, synthesis andphysical properties of metal alkoxides, development of sol-gel process from alkoxides, derived coatings, fibers and monodispersed submicron/ nanostructured oxide powders, ormosils, sialons.
***Hydrothermal/Solvothermal Approach*:** Forced hydrolysis at elevated temperatures and pressures, hydrothermal reactions using salt solutions, metal reactants and reactions involving phase transformation.

***Gas Phase Reactions*:** Gas-phase nucleation, flame hydrolyzed powders, direct - nitridation and carbothermic reduction, non-plasma gas phase reactions, plasma reactions, electron beam evaporation.

Reference Books:

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
- A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
- C. N. R. Rao and J. Gopalkrishanan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
- R. E. Newnham, *Structure Property Relations*, Springer-Verlag, 1987

CHE DET 1108: Principles of X-ray Diffraction and Electron Microscope

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Geometry of Crystal Structure

Form of solids, space lattice, seven crystal systems; unit cell, primitive and non-primitive cell,, Bravais lattice, lattice direction and crystal planes; Miller indices of crystal planes, separation between crystal planes, reciprocal lattice

Crystal Structure; closed packed structure- hcp and ccp, rack salt (NaCl), Wurzite and zinc blend of ZnS, diamond, CsCl, Fluoride (CaF_2) and antifluoride (Na_2O), Rutile (TiO_2) *etc*.

Unit – II: Point and Space Groups

Symmetry operation and symmetry elements, Plane of symmetry, inversion centre, proper and improper axis of rotation, product of symmetry operation, Relation among symmetry elements and symmetry

operation, thirty two point groups, representation of point groups with selected examples like 222, mm2, mmm, 32 centrosymmetric and non-centrosymmetric point groups.

Space group: Triclinic P1, monoclinic C2, monoclinic C2/m, orthorhombic $P222_1$ orthorhombic F222, Tetragonal 14_1, space group and crystal structure of perovskite ABO_3 and rutile structure of TiO_2 etc

Unit – III: X-ray Diffraction by Crystal

Properties of X-rays, production and detection of X-ray, diffraction of X-ray by crystal, Bragg's condition, Brag's law, diffractometer and diffractometer methods (Laue, rotating-crystal, and powder methods), Scherrer formula, scattering of an electron, atom, by a unit cell, structure factor, systematic absence, intensity of powder pattern line.

Determination of crystal structure, chemical analysis by X-ray diffraction, chemical analysis by X-ray spectroscopy (EDX energy dispersive X-ray spectroscopy).

Unit – IV: Electron Microscope

Introduction: optical microscope versus electron microscopy, brief history of electron microscope, interaction of electron and matter, elastic in-elastic scattering of electron,

Instrument: scanning electron microscope (SEM), transmission electron microscope (TEM); electron source; lenses and lenses defects, apertures and resolution, electron detection and display, pumps and sample holders, calibration of imaging system, specimen preparation for TEM

Unit – V: Transmission Electron Microscope

Forming diffraction pattern and images; principle of image contrast, bright field and dark field imaginings, and SAED and obtaining SAED, high-resolution TEM, grain boundary, phase boundary, and other imaging techniques.

Reciprocal space; diffraction from crystals; diffraction from particles, and dislocation, indexing of diffraction patterns, Kikuchi diffraction.

References Books:

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
- A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
- C. N. R. Rao and J. Gopalkrishanan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
- D. B. Williams and C. B. Carter: *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, 1996.
- B. D. Cullity: *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, 1959.

CHE DET 1109: Advanced Electrochemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I : Fundamentals of Advanced Electrochemistry

Basic electrochemistry concepts, Ideally polarizable and non-polarizable electrodes, Reference electrodes, Working electrodes, Counter electrodes, Electrified interfaces, Electrical double layer, Adsorption phenomena at electrodes, Kinetics of electron transfer, Overpotential, Exchange current density, Butler-Volmer equation – derivation and approximations, Tafel equation, Standard electrode potential, Potentiometry, Nernst equation, Modes of mass transfer, Diffusion, Faradaic vs. Non-Faradic processes, Electrolysis, Faraday's laws.

Unit – II: Electrochemical Techniques & Instrumentation

Electrochemical Techniques, Electrodeposition, Voltammetry (Cyclic Voltammetry, Linear Sweep Voltammetry), Reversible and irreversible reactions, Amperometry, Coulometry, Chronoamperometry, Chronopotentiometry, Rotating electrodes, Microelectrodes, Electrochemical Impedance spectroscopy, Spectro electrochemistry, Scanning electrochemical microscopy, Electrochemical instrumentation-simple circuits.

Unit – III: Quantum-oriented Electrochemistry

The Electrochemical potential of electrons in solution and their quantal energy states, The density of states in metals; Tunneling: The idea, equations of tunneling, tunneling through adsorbed layers at electrodes; A quantum mechanical description of electron transfer: The Frank-Condon principle in electron transfer; A quantum mechanical formulation of the electrochemical current density: equation; A retrospect and prospect for quantum electrochemistry.

Unit – IV: Applications of Electrochemistry

Introduction of Battery, Requirement for good battery, Factors affecting the capacity of battery, Major component of battery, Primary Battery: Dry (or) Laclanche cell, Alkaline battery; Secondary Battery: Lead Acid Storage Cell, Nickel-Cadmium (Ni-Cd) battery; Vanadium Redox Flow Battery, Lithium-ion Battery; Supercapacitors; Electrocatalysis; Electrochemical Sensors; Electrolysis; Electroplating; Corrosion and its prevention.

Unit – V : Fuel cells

Introduction: History of fuel cells, operating principles of fuel cells, Fuel cell types, Fuel cell applications, Fuel cell thermodynamics, Fuel cell reaction kinetics.
Polymer Electrolyte Membrane Fuel cell components, Materials, Properties and Processes: Diffusion media, Electrocatalysts, Proton Exchange membrane.
Fundamental Electrochemical Variables: Voltage, Current and Time; Basic Fuel Cell Test Station Requirements; Current-Voltage Measurements.
Transport processes in PEM fuel cells: Ion transport in an electrolyte, Electron transport, Gas-phase mass transport, Heat generation and transport.

Application in different Sectors: Stationary, transportation, space and defense sector.

Reference Books:

- Allen J. Bard & Larry R. Faulkner: *Electrochemical Methods Fundamentals and Applications,* Eds: 2nd, Wiley-India, New Delhi, 2006.
- John O'M. Bockris & Amulya K. N. Reddy: *Modern Electrochemistry, Ionics, Vol. 1,* Eds: 2nd, Springer, New Delhi, 2006.
- John O'M. Bockris, Amulya K. N. Reddy & Maria Gamboa-Aldeco: *Modern Electrochemistry, Fundamentals of Electrodics, Vol. 2A,* Eds: 2nd, Springer, New Delhi, 2006.
- D. R. Crow: *Principles and Applications of Electrochemistry,* Eds. 4th, Blackie Academic & Professional, Madras, 1994.
- James Larminie, Andrew Dicks: *Fuel Cell Systems Explained,* Wiley, 2003.
- Frano Barbir, *PEM Fuel Cells Theory and Practice,* Academic Press July 2005.
- Subramaniam Srinivasan, *Fuel Cells: From Fundamentals to Applications,* Springer, 2006.
- Gregor Hoogers: *Fuel Cell Technology Handbook,* CRC Press, Taylor & Francis Group, USA, 2002.
- David Linden, Thomas Reddy: Handbook of Batteries, Eds 3rd, Mcgraw-hill, 2002.
- G.A. Nazri, P. Balaya, A. Manthiram, A. Yamada, and Y. Yang: *Advanced Lithium-Ion Batteries Recent trends and perspectives,* Wiley-VCH.

CHE DET 1110: Polymer Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Introduction

Importance of polymers. Basic Concept: monomers, repeat units, degree of polymerization; linear, branched, and network polymers; classification of polymers. Polymerization: condensation, addition, radical, chain- ionic- and co-ordination-, and co-polymerization; polymerization condition and polymer reaction; polymerization in homogeneous and heterogeneous systems.

Unit – II: Polymer Characterization Techniques

Polydispersion-average molecular weight concept; number, weight and viscosity average molecular weights. Polydiversity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group, viscosity, light scattering, osmotic, and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers. Spectroscopic methods, X-ray diffraction, microscopy studies. Thermal analysis and physical testing tensile strength, fatigue, impact, tear resistance, hardness and abrasion resistance analysis.

Unit – III: Structure and Properties

Morphology and order in crystalline polymers – configuration of polymer chains; crystal structure of polymers; morphology of crystalline polymers; strain-induced morphology; crystallization and melting polymer structure and physical properties – crystalline melting point, T_m, melting points of homogeneous series effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g, relationship between T_m and T_g, effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Properties requirements for polymer utilization.

Unit – IV: Polymer Processing

Plastic, elastomers and fibres, compounding; processing techniques- calendaring, die casting, rotational casting, film casting, injection casting, blow moulding, extraction moulding, thermoforming, foaming, reinforcing, and fibre spinning.

Unit – V: Properties of Commercial Polymers

Polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resins, epoxy resins and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

Reference Books:

- Fred W. Billmeyer: *Textbook of Polymer Science*, Eds: 3rd, Wiley-India, New Delhi, 2012.
- A Ravve: *Principle of Polymer Chemistry*, Eds. 3rd, Springer Science + Business Media, New York, 2012.
- J. M. G. Cowie: *Physics and Chemistry of Polymers*, Blackie Academic and Professional.
- H. R. Alcock and F. W. Iamtee: *Contemporary Polymer Chemistry*, Prentice Hall.
- V. R. Govarikar, N. V. Viswanathan, and J. sreedhar: *Polymer Science*, Wieley-Eastern.

CHE DET 1111: Chemistry of Natural Products

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Alkaloid – I

Occurrence and isolation, biological role of alkaloids, General properties, nomenclature and classification of alkaloids on the basis of amino acid origin and present core structure. Isolation, properties and structural elucidation of quinine, Morphine (structure, synthesis, molecular rearrangement, stereochemistry and biogenesis).

Unit – II: Alkaloid – II

Structure and biological role of nicotine, cocaine, quinine, reserpine, vincristine, morphine, caffeine, papavarine, hyocimine. Strychnine and lysergic acid.

Unit – III: Steroid

Introduction, nomenclature of steroids, absolute configuration of steroid. Occurrence, isolation, structute elucidation and chemical properties of Cholesterol.

Unit – IV: Terpenes

Secondary metabolites: Definition and examples; terpenes – isoprene rule; mono terpenes: structure of geraneol, limonene, alpha-pinene and camphor; sesquiterpenes: longfolene;

diterpenes: abietic acid, taxol. Structure determination of Citral and Camphor.

Unit – V: Vitamins

Introduction, chemical properties, structure elucidation of Vitamin A, Vitamin B, Ascorbic Acid and Vitamin D. Vitamin A and its role in vision. Biological role of Vitamin D, Ascorbic Acid, Vitamin A.

Reference Books:

- I. L. Finar: *Organic Chemistry Vol. II*, 5th Edition
- S. V. Bhat, B. A. Nagaramgagi, M. Srikumar: *Chemistry of Natural Products*, Alpa Science International Ltd, 2005 by
- O. P. Agarwal: *Chemistry of Natural Products, Vol I & Vol II*, Goel publishing House, 1989
- J. R. Hanson: *Natural Products: The Secondary Metabolites*, Wiley-Vch, 1st Ed.

CHE DET 1112: Advanced Synthetic Organic Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Metal Mediated C-C and C-X Coupling Reactions

Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia Lythgoe olefination and Peterson's stereoselective olefination. Olefin metathesis by Ist and IInd generation catalysts: Reaction mechanism and application in the synthesis of heterocycles.

Unit– II: Reagents of Phosphorous, Sulfur, Silicon and Boron

Phosphorous Sulfur, Silicon and Boron containing compounds-preparations and their uses in organic reactions.

Unit – III: Oxidation and Reduction

***Oxidation*:** Oxidation of hydrocarbons (alkanes, aromatic hydrocarbons, alkenes), Oxidation of alcohols (Chromium reagents, Manganese reagents, Other metal and non-metal based oxidants), Oxidation of

ketones (α, β-unsaturated ketones, α-hydroxy ketones, Baeyer-Villiger oxidation of ketone)
***Reduction*:** Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents (Derivatives of lithium aluminium hydride and sodiumborohydride, mixed lithium aluminium hydride-aluminium chloride reagent, DIBAL-H, $NaBH_3CN$, sodium triacetoxyborohydride, Borane and derivatives, other methods of reductions).

Unit – IV: Disconnection Approach, Umpolung Chemistry and Protection-Deprotection of Functional groups

Basic principles and terminology-Target molecule, FGI, Disconnection, Synthon, Reagent and Retro-synthetic approach. **One group C-C and C-X disconnection**: (disconnection of alcohols, alkenes, and carbonyl compounds). **Two group C-C & C-X disconnections**: 1,3 and 1,5 difunctionalised compounds, α, β, unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels- Alder reaction, connection in retro synthesis. Umpolung in organic synthesis. Protection and deprotection for functional groups as hydroxyl, amino, carboxylic and carbonyl.

Unit – V: Some Important Organic Reactions
Selective Stereoselective Organic Reactions with Alkenes: Sharpless Asymmetric Epoxidation, Asymmetric Aziridination, Dihydroxylation, Amino-hydroxylation Reactions, Oxidative cleavages of alkenes.
Green Chemistry, Supramolecular chemistry (Crown ether, Cyclodextrin and Clalixerins) and multicomponent reactions (Ugi, Passerini, Biginelli, Hantzsch reactions).
***Chemistry of Aliphatic and Aromatic Heterocyclic Compounds*:** Epoxide, Aziridine, Azitidine, Oxetane, Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions.

References Books:

- B. F. G. Johnson: *Transition Metal Cluster*, Wiley, 1980.
- R. H. Crabtree: *The Organometallic Chemistry of the Transition Metals*, Wiley-Interscience, 2005.
- G. Wikinson, F. G. A. Stone, and E. Abel: *Comprehensive Organometallic Chemistry*, Peramon, 1980.
- I. Fleming: *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1976.
- B. B. Woodward and Hoffman: *Conservation of Orbital Symmetry*, Verlag Chemie Academic Press, 1971.
- S. Warren: *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons (Asia) Pte. Ltd., 2007
- W. Carruthers and I. Coldham: *Modern Methods of Organic Synthesis*, Fourth Ed. Cambridge University Press.
- T. L. Gilchrist: *Heterocyclic Chemistry*, Pearson Education, 3rd Ed.2007

CHE DET 1113: Advanced Heterocyclic Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Introduction
Definition of heteroatom, Aromatic and non-aromatic heterocyclic compounds, Classification and

nomenclature of heterocyclic compounds, important reactions with heterocyclic compounds i.e. oxidation, reduction and tertiary effect of Nitrogen in heterocyclic compound.

Unit – II: Non-Aromatic Heterocycles
Different types of strains, interactions and conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of the following ring systems: Aziridines, Oxiranes, Thiiranes, Oxaziridines, Azetidines, Oxetanes and Thietanes.

Unit – III: Five and Six Membered Heterocyclics with One Hetero Atom
Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions [Advanced level Synthetic preparation or method applied].

Unit – IV: Five and Six Membered Heterocyclics with Two Hetero Atoms
Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

Unit – V: Larger Ring and Other Heterocycles
Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Benzoazepines, Benzooxepines, Benzothiepines, Azocines and Azonines.

Reference Books:

- T. Gilchrist: *Heterocyclic Chemistry*
- R. M. Acheson: *An Introduction to the Chemistry of Heterocyclic Compounds*
- J. A. Joule & K. Mills: *Heterocyclic Chemistry*
- A. Paquette: *Principles of Modern Heterocyclic Chemistry*
- J, A. Joule & Smith: *Heterocyclic Chemistry*
- A .R. Katritzky: *Handbook of Heterocyclic Chemistry*

CHE DET 1114: Bioorganic and Drug Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Overview of Bioorganic Chemistry
***Introduction*:** Definition of bioorganic chemistry, Border line of bioorganic chemistry and inter disciplinary area between chemical and biology, Weak interaction in organic and biological world, Molecular Recognition.
***Chemistry of the Living Cell*:** The structure of prokaryotic and Eukaryotic cells, Composition of living cells:

Unit – II: Carbohydrates, Proteins, Lipids, and Nucleic Acids
***Carbohydrates*:** Introduction, Reactions of Monosaccharides, Interconversions, Ring structure of aldoses and ketoses, Confirmation of Monosaccharides, Disaccharides: Structure, synthesis and properties.

***Proteins*:** General structure & classification of amino acids, Abbreviation of amino acids, Essential and non essential amino acids, Synthesis of amino acids, Isoelectric point, Acid and base properties of amino acids. Protein: Naturally occurring peptides, Modern methods of peptide synthesis with protection and deprotection, Determination of sequences and basic units of a poly peptides or proteins, C- & N-terminus detection by chemical methods, Primary, secondary, tertiary and quaternary structures of proteins, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases etc.

***Lipids*:** Lipid structure- acylglycerols, phosphoglycerides and sphingolipids, Biological importance of fatty acids and lipids, Bio- and chemical Synthesis of lipids.
***Nucleic Acids*:** Definition, structure and properties, base pairing, double helices, Genetic information storage, transmission and gene expression, Nucleotides and Nucleosides: Similarities and differentiation, Structure of DNA & RNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis.

Unit – III: Analogy Between Biochemical and Organic reactions
Introduction to metabolism (catabolism, anabolism). ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD^+, FAD. Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle. Overview of catabolic pathways of fat and protein. Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types.

Unit – IV: Overview of Drug Chemistry and Basics of Drug Action
Definition, classification and nomenclature of drugs, Preliminary idea of drug action: Interaction (Weak interaction in drug molecules, Chirality and drug action), Receptorology (Drug-receptor interactions, Enzyme kinetics in drug action, Enzyme inhibitors (Drug action through enzyme inhibition), Nucleic acids as targets for drug actions, NA-Alkylation, NA-strand breaking and their importance in drug action, Drug metabolism, drug deactivation and elimination.

Unit – V: Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

Reference Books:

- L. Stryer: *Biochemistry*, 4th Edition W. H. Freeman and Co. 1995.
- S. Zubay: *Biochemistry*, Addison-Wesely 1983.
- J. Mann; R.S. Davidson: *Natural Products: Chemistry and Biological Significance*
- H. Dugas: *Bioorganic Chemistry Frontiers Vol. 2*, ed. Springer-Verlag, 1990.
- E. E. Tamlen: *Bioorganic Chemistry*, Academic Press, 1977.
- M. Bodansky: *Peptide Chemistry: A Practical Textbook*, Springer-Verlag 1988.
- *Bioorganic Chemistry: A chemical approch to enzyme action*, Springer-Verlag 1989.
- W. Saenger: *Principles of Nucleic acid structures*, Springer-Verlag 1984.
- G. R. Chatwal: *Medicinal Chemistry*

- A. Kar: *Medicinal Chemistry*, Wiley, 2000.
- D. Lednicer: *Strategies for Organic Drug Synthesis and Design*, John Wiley 1998.
- G. R. Chatwal: *Synthetic Drugs*, Himalaya, New Delhi 1995.
- S. Hanessian, *Total synthesis of Natural product: The chiral approach Vol.III* Pergamon Press 1983.
- W. D. Foye, T. L. Lemke, and D. A. Williams: *Principles of Medicinal Chemistry (*4th Edition)
- R. B. Siwerman: *Organic Chemistry of Drug Action and Design* (Academic press, 1993).

CHE DET 1115: Molecular recognition and Supramolecular Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Principal of molecular recognition

Concept of molecular recognition and Supramolecular Chemistry. Host-Guest Chemistry, and its classification. Receptor, Coordination and the lock and key analogy. Thermodynamic and Kinetic Selectivity. Nature of supramolecular interactions.

Unit – II: Supramolecular Chemistry of Life

Alkali metal ions in biochemistry. Porphyrins and Tetrapyrrole macrocycles. Plant Photosynthesis. Uptake and transport of oxygen in Haemoglobin. Coenzyme B_{12}.Neurotransmitter and Hormones. DNA. Biochemical self assembly.

Unit – III: Cation & Anion Binding Host

Crown ether, Lariat ether and podands, Cryptands, Calix[n]arenes; Spherands; Selectivity of cation complexation; Macrocyclic, Macrobicyclic and Template effect.

Concept of Anion binding host design. Guanidium-based receptors; Organometalic receptors; Neutral receptors, Hydride sponge; Anticrown; Biological anion receptors.

Unit – IV: Binding of Neutral molecules

Binding by cavitands, cyclodextrines, Molecular cleft and tweezers, cyclophanes, cryptophanes Host.

Unit – V: Supramolecular reactivity and Catalysis

Catalysis by cation, anion and neutral receptors; Supramolecular metallocatalysis; Cocatalysis; Biomolecular and abiotic catalysis.

Reference Books:

1. J. W. Steed and J. L. Atwood: *Supramolecular Chemistry*, John Wiley and Sons, Ltd.
2. Jean –Marie Lehn: *Supramolecular Chemistry-Concepts and Perspectives*, VCH.
3. Hans-Jorg Schnider and Anatoly K. Yatsimirsky: *Principles and Methods in Supramolecular Chemistry*, John Wiley and Sons, Ltd.
4. Antonio Bianchi, Kristin Bowman James and Enrique Garcia-Espana: *Supramolecular Chemistry of anions*, Wiley-VCH.

CHE DEP 1116: Chemistry Practical

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

Advanced Analytical Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

Group-A: Analysis of Complex Materials

Quantitative analysis of complex materials, such as, ores and minerals, metals and alloys, industrial materials by conventional and or instrumental methods as applicable.

Model Samples

Ores, Minerals , Concentrates*:* Dolomite ($CaCO_3$, Mg CO_3, Fe_2O_3, SiO_2); Pyrolusite (MnO_2, MnO, Fe_2O_3); Chalcopyrite (CuS, FeS); Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2); Chromite (Cr_2O_3, Fe_2O_3, MnO, SiO_2); Basic slag (Al_2O_3, Fe_2O_3, P_2O_5, SiO_2).

Metals and Alloys: Brass (Cu, Zn); Soldier / Type metal (Pb, Sb, Sn); Bronze(Cu, Zn, Sn), Aluminium bronze(Cu, Al, Fe, Mn), Steel (Cr, Mn, Ni, P).

Mixture: Chromium (III) and Mn(II) in a mixture, Iron (III) and Cu(II) in a mixture, Iron(III) and Al(III) in a mixture

At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session.

Group-B: FT-IR and UV assignment of synthesized metal complexes

Group-C: Presentation / Seminar

Group-D: Literature Review report

Reference Books:

- I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Gary D. Christian: *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.

Advanced Organometallic Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

A. Preparation of selected inorganic compound and their studies by I.R., electronic spectra, Mössbauer and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds

1. Mn_{12} Acetate Single Molecule Magnets

2. $K_2[Fe(C_2O_4)_3]$ .3 H_2O
3. $[Fe_3(\mu_3\text{-}O)(\mu\text{-}O_2CR)_6L_3]$ (L = H_2O, R= alkyl/aryl/)
4. $[Fe_3O(PhCO_2)_6(MeOH)_3](NO_3)(MeOH)_2$
5. $[Fe_8O_3(O_2CCMe_3)_6(N_3)_3(tea)(teaH)_3]\cdot 0.5(EtOH)$
6. $Cu_2(C_6H_5COO)_4(C_6H_5COOH)_2$
7. Tris(ethylenediamine)nickel(II) thiosulphate

B. Determination of crystal Structure by ORTAP file.
C. Presentation / Seminar
D. Literature Review report

References Books:

- Liz, T. *Acta Crystallogr.* ***1980***, *B36*, 2042
- Sessoli, R.; Tsai, H.-L.; Schake, A. R.; Wang, S.; Vincent, J. B.; Folting, K.; Gatteschi, D.; Christou, G.; Hendrickson, D. N. J. Am. Chem. Soc. 1993, 115, 1804.
- J-X. Daia, F-H. Wua, A. Rothenbergerb, Q-F. Zhang, *Z. Naturforsch.*, 2007, 62b, 1117 – 1122.
- M. K. Zart, D. Powell, A. S. Borovik, *Inorganica Chimica Acta*. 2007, 360(7), 2397–2402.
- V. Psycharis, C. P. Raptopoulou, A. K. Boudalis, Y. Sanakis, M. Fardis, G. Diamantopoulos, G. Papavassiliou, *Eur. J. Inorg. Chem.*, 2006, 3710–3723.
- M. Narshim, A. Saritha, B. Raju, K. A. Hussain, IJIRSET, 4(8), 2015, 7548-7555.
- Olga Botezat, Jan van Leusen, Victor Ch. Kravtsov, Arkady Ellern, Paul Kögerler and Svetlana G. Baca, Dalton Trans., 2015, 44, 20753.
- S. Pathak, N. Biswas, B. Jana, T. K. Ghorai, Advanced Materials proceeding, 2017

Modern Physical Methods in Chemistry Research/Advanced Materials Chemistry/Principles of X-ray Diffraction and Electron Microscopy/Advanced Electrochemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

1. Synthesis: A) Solid State method, (Fe_2O_3/TiO_2, Fe_2O_3/ZnO, Fe_2O_3/ZrO_2)

   B) Co-precipitation (transition metal doped ZnO, ZrO_2)

   C) Green Technique: Ag Nanoparticles, Cu NPs, Zn NPs etc.

   D) Sol-gel: ZnO, ZrO_2

   E) Synthesis of Graphene oxide nano powder

F) Synthesis of Carbon nano tube

G) Synthesis of nanoparticles using electrochemical methods

2. Characterization: UV, FTIR, XRD, Electron Microscopy (available of Department)
3. Application Study: Optical, Magnetic, Catalytic etc.
4. Presentation / Seminar
5. Literature Review report

Reference Books:

- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).
- G. L. Hornyak, J. J. Moore, H. F. Tibbals, and J. Dutta: *Fundamentals of Nanotechnology*, CRC Press, 2009

Polymer Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

1. Polymer Synthesis:

i) Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).
Purification of monomer
Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutylonitrile (AIBN)

ii) Preparation of nylon 66/6
iii) Redox polymerization of acrylamide
iv) Precipitation polymerization of acrylonitrile
v) Preparation of urea-formaldehyde resin
vi) Preparations of novalac resin/resold resin.

2. Polymer characterization

i) Determination of molecular weight by viscometry:
Polyacrylamide-aq.$NaNO_2$ solution
ii) Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.
iii) Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

3. **Polymer analysis**

i) Estimation of the amount of HCHO in the given solution by sodium sulphite method

ii) Instrumental Techniques
iii) IR studies of polymers
iv) DSC analysis of polymers
v) Preparation of polyacrylamide and its electrophoresis

4. **Presentation / Seminar**

5. **Literature Review report**

Reference Books:

- Malcohm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
- Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
- Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
- Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
- L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)
- Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

Chemistry of Natural Products/Advanced Synthetic Organic Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

A. Extraction

1. Extraction of caffeine from tea leaves.
2. Lycopene extraction form Tomatoes
3. Extraction of DNA from onion/cauliflower
4. Separation of amino acids by paper chromatography
5. Study of titration curve of glycine
6. To determine the saponification value of an oil/fat.
7. To determine the iodine value of an oil/fat
8. Practical Synthesis of of any one indole alkaloids.
9. If possible, extraction of any alkaloids from plants.

B. **Synthesis of Organic Compounds**:

1. Pd-catalyzed Heck reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

1. Pd-catalyzed Suzuki coupling reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

2. Pd-catalyzed Sonogishira coupling reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

3. Wittig reaction and Wittig Horner method for alkene synthesis (Any one suitable example from each reaction).

4. Oxidation and Reduction (choose any one suitable example from each category)

(i) Oxidation of secondary alcohol to ketone
(ii) Oxidation of primary alcohol to aldehyde
(iii) Reduction of aldehydes by $NaBH_4$
(iv) Reduction of ketones by $LiAlH_4$

5. Synthesis of an Imidazolidinone Organocatalyst and its application in a DA Reaction: Multistep Synthesis

(i) Catalyst synthesis
(ii) Diels-Alder reaction.
(iii) Purification step
(iv) Spectral data analysis (1H-NMR and 13C-NMR)

6. Multi component reaction: Biginelli reaction

Advanced Heterocyclic Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

1. Three member Heterocycles:
i) Epoxide synthesis from alkenes
ii) Epoxide synthesis from Halohydrin substrates
iii) Aziridination of alkenes
iv) Aziridine synthesis from amino acids
2. Five member Heterocycles:
i) Hantzsch synthesis of Pyrrole.
ii) Multicomponent reaction for synthesis of Pyrrole (Jana method).
iii) Meyer's Oxazoline synthesis from amino alcohol.
3. Fused five- or six member heterocycles:
i) Indole synthesis
ii) Quinoline synthesis
iii) Synthesis of 1-Phenyl-1,2,3,4-tetrahydroisoquinolines.
4. Basic reactions with heterocycles:
a) Treatment of Br_2 in MeOH and followed by oxidation with Amberlyst-15.
b) [3+2]-cycloaddition reaction of aziridine and carbonyl compounds in the presence of Lewid acid.

References of Books:

- *Practical Organic Chemistry* by A. I. Vogel.
- *Practical Organic Chemistry* by F. G. Mann and B. C. Saunders.
- The Organic Chemistry Journals: plz search Supporting informations of Journal of Organic chemistry, Organic Letters and Journal of American chemical Society from ACS Publication and Angew. Chem.

Int. Ed. (Willey publishers); Chemical Communication (Royal Chemical Society) for appropriate experimental methods.

- *Journal of Chemical Education* **1985**, *62*, 262.

Bioorganic and Drug Chemistry/Molecular Recognition and Supramolecular Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

(a) Synthesis of Following Drug Molecules:

1. Paracetamol
2. Acetanilide
3. Aspirin
4. Phenazone
5. Ibuprofen

(b) Synthesis of short peptide containing 2-3 different amino acids.

(c) Craracterization:

1. Practices for recording the UV-visible spectra of suitable chromophoric molecules.
2. Sample preparation and recording the IR Spectra for IR-active compounds.
3. Analyze the first-order/ second order ^{1}H-NMR Spectra of any standard organic molecules (Identification of chemical shifts for all protons, measurement of coupling constant, diastereoisomers ratio, determination of chemical yields by using a standard)
4. Analyze the 2D-^{13}C-NMR spectra of any organic molecules.
5. Analytical separation of diastereoisomers and enantioisomers by using HPLC techniques and determining the enantiomeric purity (ee/er) and diastereoisomers ratio (d.r.) by HPLC chromatogram.

After completion of above hands on experiences, a student would be enabling to analyze any unknown spectroscopic datas (e.g.; UV-Visible spectra, IR Spectra, 1H-NMR spectra and 13C-NMR Spectra).

References of Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry,* R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H. Freeman & Co.: New York (2003).
- Bessler and Silverstein, Spectroscopy of Organic Compounds, JOHN WILEY, 2001.
- D. C. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, *3rd Edition*, THOMSON, 2007.
- Organic Spectroscopy III Edition–by William Kemp
- *Practical Organic Chemistry* by A. I. Vogel.
- *Practical Organic Chemistry* by F. G. Mann and B. C. Saunders.
- For Pd-catalyzed cross coupling reaction, recommend ACS journal's Supporting Information
- *J. Chem. Edu.* (DOI: 10.1021/acs.jchemed.5b00812)
- *Advanced Practical Organic Chemistry* by J. Leonard, B. Lygo and G. Proctor.

COURSES OF STUDIES

FOR POST GRADUATE DEGREE IN CHEMISTRY
(SEMESTER SYSTEM)

Session: 2023-24

DEPARTMENT OF CHEMISTRY
INDIRA GANDHI NATIONAL TRIBAL UNIVERSITUY
AMARKANTAK, MADHYA PRADESH-484887

Programmes/ courses focused on employability/ entrepreneurship/ skill development during the Academic year

FIRST SEMESTER

PAPER CODE: CHM T 411: PHYSICAL CHEMISTRY –I

SYLLABUS

Unit – I: Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential, and entropies. Thermodynamics of open systems: partial molal properties, partial molal free energy, partial molal volume and partial molal heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity. Non-ideal system: excess function for non-ideal solutions. Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solution; determination of activity and activity coefficients; ionic strength.

Unit – II: Heterogeneous Catalysis

***Heterogeneous Catalysis* (*Surface Reactions*):** Kinetics of uni-molecular reactions- inhibition and activation energy. Bimolecular surface reactions - reactions between a gas molecule and an adsorbed molecule, reaction between two adsorbed molecules. Effect of temperature on surface reaction promoters and poisons.

Unit – III: Homogeneous Catalysis

Kinetics Homogeneous Catalysis: Nature of surface, concept of active centers. Kinetics of enzymatic reactions: Michaelis-Menten equation, Lineweaver-Burk and Eadie Analyses, enzyme inhibition (competitive, non-competitive and uncompetitive inhibition), effect of temperature and pH of enzymatic reaction; acid – base catalysis and their mechanism.

Unit – IV: Electrochemistry

***Electrochemistry of Solution*:** Debye-Hückel treatment and its extension, ion solvent interaction. Debye-Hückel-Jerum mode. Thermodynamics of electrified interface equation. Derivations of electrocapillary, Lippmann equation (surface excess); method of determination structure of electrified interfaces. Gouy-Chapmann, Stern, Graham-Devanathan Mottwatts, Tobin, Bockris, Devanathan Models.

Over Potential: Exchange current density, derivation of Butler-Volmer equation, Tofel plot. Quantum aspect of charge transfer at electrodes-solution interfaces, quantization of charge transfer, tunneling.

Corrosion: Introduction to corrosion, homogeneous theory, forms of corrosion, corrosion monitoring and prevention method.

Unit – V: Surface Chemistry

***Surface Tension*:** Capillary action, pressure difference across curved surface (Laplace equation), vapor pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, estimation of surface area (BET equation), surface film and liquids (electro-kinetic phenomenon), catalytic activities at surface.

***Surface Active Agents*:** Classification of surface-active agents. Micellization, hydrophobic interaction, critical micellar concentration (CMC), factor affecting the CMC of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro-emulsion reverse micelles.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 412: INORGANIC CHEMISTRY –I

(Transition and Inner Transition Metal Chemistry)

SYLLABUS

Unit – I: Co-ordination Chemistry

Experimental evidence of metal-ligand overlap, spin orbit coupling constant and interelectronic coupling parameters in complex ion terms-vs-free ion terms, Nephelauxetic effect, *d*-orbital splitting in octahedral, Jahn-Teller distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes, CFSE for d^1 to d^{10} systems, pairing energy, low-spin and high-spin complexes and magnetic properties, Crystal field activation energy, hole formalism, Tetrahedral distortion and Jahn Teller effect, Static and Dynamic Jahn-Teller effect, Effect of crystal field stabilization on ionic radii, lattice energy, hydration enthalpy and stabilization of complexes (Irving Williams order). Colour and spectra, Kinetic aspects of crystal field stabilization. Adjusted CFT, Limitations of CFT, Labile and inert complexes.

Unit – II: Electronic Spectra of Transition Metal Complexes

Microstates, Russell-sander's terms, determination of ground and excited state terms of d^n ions; Orgel diagrams (qualitative approach) and Tanabe-Sugano diagram, selection rules for spectral transitions, *d-d* spectra of d^n ions and crystal field parameters, Nephelauxetic series, Electronic Spectra UV-Vis, charge transfer, colors, intensities and origin of spectra. MOT to rationalize σ and π interactions in octahedral, square planar and tetrahedral metal complexes. Symmetry designations of LGOs and MOs. Simplified MO diagrams.

Unit – III: Magneto Chemistry

Basic principles of magnetism, Magnetic properties, paramagnetism, ferro- and antiferro magnetism, diamagnetism, Pascal constants, Currie equation, determination of magnetic susceptibility, application of Van Vleck susceptibility equation, Magnetic properties and coordination compounds Spin and orbital moments, spin – orbit coupling, quenching of orbital moment, spin only formula, room temperature and variable temperature magnetic moments and spin crossover. Magnetic properties of first transition series metal ions, lanthanides and actinides, Lanthanide and actinide contractions and their consequences, separation of lanthanides and actinides and their applications (examples). Magnetic exchange interactions. ESR spectroscopy, Basic concept of Single Molecule Magnets (SMM), properties, examples and application of SMMs.

Unit – IV: Inorganic Reaction Mechanism

Mechanism of substitution reactions, solvent exchange, aquation, anation, base hydrolysis, acid catalyzed aquation, pseudo-substitution. Energy profile diagram of ligand substitution reactions- associative (A), dissociative (D), interchange (I) etc. type pathways, relation between intimate and stoichiometric mechanisms of ligand substitution, some important rate laws, activation parameters ($\Delta S^{\#}$, $\Delta H^{\#}$, $\Delta V^{\#}$), mechanism of isomerization reaction-linkage isomerism, cis-trans isomerism, intramolecular and intermolecular racimization, Ray-Dutta and Bailar twist mechanisms, substitution in octahedral complexes- the Eigen-Wilkins mechanism, the Fuoss-Eigen equation, linear free energy relation (LFER) etc. Mechanism of electron transfer reactions: General characteristics and classification of redox reactions, self-exchange reactions. Frank-condon principle (non mathematical treatment). Outer sphere and Inner sphere reactions, applications of Marcus expression (simple form), redox catalyzed substitution reactions.

Unit - V: Chemistry of Elements

d-Series Elements: Electronic configuration, oxidation states; aqueous, redox and coordination chemistry, spectral and magnetic properties of compounds in different oxidation states, horizontal and vertical trends in respect of 3d, 4d, and 5d elements with references to Ti-Zr- Hf , V-Nb-Ta, Cr- Mo- W, Mn-Tc-Re and Pt group metals. Occurrence and isolation in respect of V, Mo, W, Re, Pt. Iso- and heteropolyoxometalates with respect to V, Mo, and W: synthesis, reactions, structures, uses, metal-metal bonded dinuclear d-metal complexes (examples), bonding in dirhenium complexes.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 413: ORGANIC CHEMISTRY –I

(Organic Reaction Mechanism and Stereochemistry)

SYLLABUS

Unit – I : Physical Organic Chemistry

Thermodynamic and kinetic requirements of a reaction: Transition state theory, Hammond's postulate, Kinetic vs Thermodynamic control
Acids and Bases
Determining the mechanism of a reaction: Detection and trapping of intermediates, Cross-over experiments, kinetic isotopic effect-primary kinetic and secondary kinetic isotopic effect

Unit – II: Substitution, Addition, and Elimination Reactions

Substitution Reaction: Aliphatic nucleophilic substitution- SN1, SN2, SNi mechanism, classical and nonclassical carbocations, phenonium ions, NGP-in substation reactions. Effect of solvent, structure, nucleophile and leaving group on rate of SN1, and SN2 reaction. Electrophilic aromatic substitution and Nucleophilic aromatic substitutions. Mechanism and stereo chemical aspects of substitution reactions.
Addition Reaction: Addition to carbon-carbon multiple bonds, addition to carbon-heteroatom multiple bonds, electrophilic, nucleophilic and free radical addition reactions. Mechanism and stereo chemical aspects of addition reactions.
Elimination Reaction: E1, E2, E1cb mechanisms, orientation and stereochemistry in elimination reaction, reactivity effect of structure, attacking and leaving group, competition between elimination and substitution, syn-eliminations.

Unit – III: Symmetry Operation and Stereoisomerism

Simple or proper axis of symmetry, plane of symmetry, centre of symmetry and improper or rotation-reflection of symmetry. Enantiomerism and diastereomerism, conventions for configurations D-L and R-S systems, Threo and erythro nomenclature. Measurement of optical purity, enantiomeric excess. Stereoselective and Stereospecific reactions. Molecules with tri- and tetra coordinated chiral centres. Molecules with two or more chiral centres.

Unit – IV: Chirality and Conformations

Axial and Planar Chirality: Principles of axial and planar chirality. Stereochemistry of allenes, Stereochemistry of biphenyl derivatives and atropisomers. Stereochemistry of spiranes, Stereochemistry of molecules with planar chirality, Helicity.
Conformations & Stereoisomerism of Acyclic and Cyclic Systems: Molecular mechanics and conformations, Conformations of a few acyclic molecules, Conformations of cyclic systems: monocyclic compounds (mono, di- and poly substituted cyclohexanes); Conformations of fused ring and bridged ring compounds.

Unit – V: Dynamic Stereochemistry

Conformation and Reactivity: Conformation, reactivity and mechanism: Cyclic systems (Nucleophilic

substitution reaction at ring carbon, Addition reaction to double bonds, Elimination reactions, NGP reactions). Conformation, reactivity and mechanism: Acyclic systems (addition, Elimination and NGP participation). Formation and reaction of enols and enolates. Reduction of cyclohexanes with hydride reagents.

Stereoselective Reactions: Principle of stereoselectivity, asymmetric synthesis and asymmetric induction, Acyclic stereoselections (addition of nucleophiles to carbonyl compounds, aldol reactions, addition to allyl metal and allyl boron compound to carbonyl compounds), Diastereoselections in cyclic systems (Nucleophilic addition to cyclic ketones, alkylations, catalytic hydrogenations).

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM P 411: INORGANIC CHEMISTRY PRACTICAL - I

SYLLABUS

A. Qualitative Analysis Semi-micro qualitative analysis of mixture containing eight radicals including two less common metal from among the following:

(1) *Basic Radicals*: Ag^{+}, Pb^{2+}, Bi^{3+}, Cu^{2+}, Cd^{2+}, As^{3+}, Sb^{3+}, Sn^{4+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}, Ce^{3+}, Th^{4+}, Zr^{4+}, W^{6+}, Te^{4+}, Ti^{4+}, Mo^{6+}, V^{5+}, Be^{2+}.

(2) *Acid Radicals* : Carbonate, Sulphite, Sulphide, Nitrite, Nitrate, Acetate, Fluoride. Chloride, Bromide, Iodide, Sulphate, Borate, Oxalate, Phosphate, Silicate, Thiosulphate, Ferrocyanide, Ferricyanide, Thiocyanide, Chromate, Arsenate and Permanganate.

B. Chromatographic Separation

Use paper chromatography to separate and identify the metal ion components of an unknown solution. Chromatographic separation of sugars, amino acids by paper, T.L.C. and Ion exchange.

C. Standard Deviation

Calculation of standard deviation from the results obtained by redox titration of Fe(III) against standard solution of $K_2Cr_2O_7$.

Calculation of standard deviation from the results obtained by complexometry method of hardness (Ca^{2+}) of water using EDTA.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM P 412: ORGANIC CHEMISTRY PRACTICAL - I

SYLLABUS

Part A: Techniques of Separation and Purification

- Fractional Distillation of a mixture of liquids
- Distillation under reduced pressure
- Chromatographic separation (Paper chromatography and Thin Layer Chromatography)

Part B: Analysis of Organic Binary Mixture

Separation and Identification of organic compounds from the given binary mixtures. (Complete study of determination of organic compound with melting point and preparation of a suitable derivative)

Part C: Preparation of Organic Compounds (Single Stage Preparation)

Representative reactions to be covered:

- Electrophilic aromatic substitution reaction (Friedel-Crafts Reaction, halogenation, nitartion and sulphonation reaction)
- Acetylation reaction
- Diels-Alder reaction
- Condensation reaction
- Cannizzaro reaction
- Oxidation reaction
- Reduction reaction
- Rearrangement reaction
- Esterification
- Diazotization reaction
- Sandmeyer reaction

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

SECOND SEMESTER

PAPER CODE: CHM T 421: PHYSICAL CHEMISTRY –II

(Quantum-, Statistical- Mechanics, Symmetry & GroupTheory)

SYLLABUS

Unit – 1: Quantum Chemistry – I

***Historic Background*:** Important historic background of quantum mechanics versus classical mechanics, wave particle duality, Heisenberg's uncertainty principle.

***Schrödinger Wave Equation*:** normalization and orthogonality of wave functions; time-dependent and time-independent Schrödinger equations.

***Operators*:** Operators and their algebra, linear and Hermitian operators, matrix representation, commutation relationship, quantum mechanical operators for position, linear momentum, angular momentum, total energy, eigenfunctions, eigenvalues and eigenvalue equation; expansion of arbitrary state in term of complete set, postulates of quantum mechanics.

Solution of the Schrödinger Equations for Some Exactly Soluble Systems: particle-in-a-box; particle-in-a-ring and -sphere; harmonic oscillator; tunneling one dimensional potential barrier and well.

Unit – 2: Quantum Chemistry – II

Rigid Rotor, spherical coordinates Schrödinger wave equation in spherical coordinates, separation of the variables, the phi equation, wave-function, quantum number, the theta equation, wave function, quantization of rotational energy, spherical harmonics.

***Hydrogen and Hydrogen Like Atoms*:** Radial and angular probability distributions, atomic orbitals.

***Angular Momentum*:** Basis functions and representation of orbital angular momentum operators, eigenfunctions, and eigenvalues of orbital angular momentum operator, Ladder operator, Spin, spin angular momenta, coupling (orbital and spin) of angular momentum, Clebsch-Gordan coefficients and Wigner Eckart theorem.

***Approximate Methods of Quantum Mechanics*:** Variational principle; time-independent perturbation theory up to second order in energy for non-degenerate and degenerate system with simple examples; application to the two electron system such as, He and He like atoms.

Unit – 3: Atomic Structure and Spectroscopic

Many electron atoms, Pauli antisymmetry principle, Hund's rules; Slater determinant; Hatree and Hatree-Fock self consistent field model for atom; electronic term symbol (Russell-Saunders and jj coupling) for atoms and spectroscopic states (selection rules for atomic spectra).

Unit – 4: Statistical Thermodynamics

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging; conical, grand conical and micro-canonical ensembles. Boltzmann distribution laws (using Lagrange's method of undetermined multipliers). Partition function –

translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in term of partition function, Applications of partition functions.

Heat capacity behavior of solid – chemical equilibria and equilibrium constant in term of partition function. Fermi-Dirac statistics, distribution law and application to metal, Bose-Einstein statistics, distribution law and application to helium.

Unit – 5: Symmetry & Group Theory

symmetry elements and symmetry operations; point groups, Schoenflies notation for point group, representation of group by matrix, character of a representation, reducible and irreducible representation, great orthogonality theorem and its importance.

Application of group theory to atomic orbitals in ligand fields, molecular orbitals, and hybridization. Selection rules for IR and Raman spectra, procedure for determining symmetry of normal modes of vibration - hybrid orbitals in BF_3, CH_4, NH_3, H_2O and SF_6.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 422: INORGANIC CHEMISTRY –II

(Chemistry of Organometallics)

SYLLABUS

Unit – 1: Organometallics – I

Organo transition metal chemistry: History, Nature of metal – carbon bonding and definition and classification of organometallic compounds, classification ligands, kinetic and thermodynamic stability of organometallic compounds. Compounds with metal carbon σ and multiple bond: Heptacity complexes of Metal-alkyl, -allyl, aryl, -carbene (Fischer and Schrock type), -carbonyl, -carbines and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity and decomposition pathway, Reactions in organometallic compounds. Stucture and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_2H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, techniques of study.

Unit – 2: **Organometallics – II**

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Catalysis by organometallic compounds: Hydrogenation of olefins, Wilkinson's catalyst, Tolman catalytic loop; synthesis gas, water-gas shift reaction; Hydroformylation (oxo process), Monsanto acetic acid process, Wacker process; synthetic gasoline: Fischer-Tropsch process and Mobile process, polymerization, oligomerization and metathesis reactions of alkens and alkynes, Zieglar- Natta catalysis, photo dehydrogenation catalyst (platinum POP).

Unit – 3: Inorganic Rings, Cages and Clusters

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds- Lipscomb's topological models, Wade`s rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

Unit – 4: New Developments in Organometallics Chemistry Research

Construction, structure and property of compounds with specific topology in Organometallic Chemistry: Capsules, boxes, containers, prisms or clusters, tubes, catenanes, rotaxanes, incorporation of metal atoms through metal-ligand coordination interactions, Various organic ligands containing carboxy, imidazole or pyridine groups, which can coordinate with metal atoms, have been used to generate the desired compounds (V, Cr, Mn, Fe, Co, Ni, Cu). Particularly, flexible ligands with central aromatic core and imidazol-1-ylmethyl pendant arms, e.g. 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene and its analogues, Interesting properties: olecular recognition, ion inclusion and exchange of these compounds, especially of the cage-like compounds, are described.

Unit – 5: Metal – ligand equilibria in solution

Stability of mononuclear, polynuclear and mixed ligand complexes in solution. Stepwise and overall formation constants and their relations. Trends in stepwise formation constants, factors affecting the stability of metal complexes with reference to the nature of the metal ions and ligands. Statistical and non-statistical factors influencing stability of complexes in solution. Stability and reactivity of mixed ligand complexes with reference to chelate effect and thermodynamic considerations. Macrocyclic and

template effect. Spectrophotometric and pH metric determination of binary formation constants.

“Employability” Green Color/ “Entrepreneurship” Blue Color/ “Skill development” Red Color

PAPER CODE: CHM T 423: ORGANIC CHEMISTRY –I I

(Principle of Organic Synthesis and Organic Spectroscopy)

SYLLABUS

Unit – 1: Principles of Organic Synthesis

***Acid Catalyzed Carbon-Carbon Bond Formation Reaction*:** Principles, Self condensation of alkenes, reactions of aldehydes and ketones, Friedel-Crafts reactions, Prins reaction and Maanich reaction and Nef Reaction.

***Base Catalyzed Reactions* (*Enolate Chemistry*):** Enolates: structure and stability of enolates, Generation of enolates using Nucleophilic and non Nucleophilic bases. Kinetic and Thermodynamic control of regioselectivity of enolates, Reactions of enolates. Alkylation and acylation of enolates: Haloform reaction, HVZ reaction, Claisen condensation, Enolate of active methylene compounds and corresponding alkylation reactions, Michael addition, Robinson annulations reaction.

Unit – 2: Rearrangement and Organometallic Reactions

***Rearrangement Reactions*:** Demjanov, Pummerer, Dienone-phenol rearrangement, Pinacol-Pinacolone rearrangement, Fries rearrangement,Wagner-Meerwein Rearrangement, Benzil-Benzilic Acid Rearrangement, Beckmann Reaction, Curtius, Schmidt, Lossen, Hoffman and Claisen rearrangement. Brook, Favorski, Neber, Von Richter, Sommelet Hauser and Wittig rearrangement.

***Organometallic Reagents*:** Organomagnesium and Lithium reagents (Preparations, uses and applications), uses of Organomercury, organocadmium, organozinc and organocopper compounds.

Unit – 3: Ultraviolet and Infrared Spectroscopy

***Ultraviolet Spectroscopy*:** Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, solvent polarity. Calculation of absorption maxima by Woodward-Fieser Rules (using Woodward-Fieser tables for values for substituent's) for the following classes of organic compounds: conjugated polyenes (cyclic and acyclic), enones and substituted benzene derivatives.

***Infrared Spectroscopy*:** Fundamental, overtone and combination bands, vibrational coupling, important group frequencies for the common functional groups.

Unit – 4: Nuclear Magnetic Resonance and Mass Spectroscopy

***Nuclear Magnetic Resonance Spectroscopy*:** Chemical shift, Factors affecting chemical shift, Chemical and magnetic equivalence, Spin-spin coupling, Coupling constant J, Factors affecting J, Karplus equation, First order spectra, Geminal, vicinal and long range coupling (allylic and aromatic). ^{13}C NMR, Heteronuclear coupling, 2D NMR spectroscopy.

***Mass Spectrometry*:** Molecular ion peak, base peak, isotopic abundance, metastable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), McLafferty rearrangement, Retro-Diels-Alder reaction, ortho effect.

Unit – 5: Structure Determination of Organic Compounds

Structure determination involving individual or combined use of the above spectral techniques.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM P 421: PHYSICAL CHEMISTRY PRACTICAL – I

A. SYLLABUS

(i) Chemical Kinetics
(a) Kinetics of Reaction between ferric nitrate and potassium iodide using initial reaction rates.
(b) Determination of the rate constant for the decomposition of hydrogen peroxide by Fe^{3+} and Cu^{2+} ions.
(c) Flowing clock reactions (Experiments in physical Chemistry by Shoemaker).

(ii) Determination of CMC of the surfactant/CMC Concentration.

(iii) Determination of partial molal volume.

(iv) Determination of the isotherm for a three component system.

(v) (a) Spectrophotometric determination of acid dissociation constant.
(b) Formula and stability constant using spectrophotometry.

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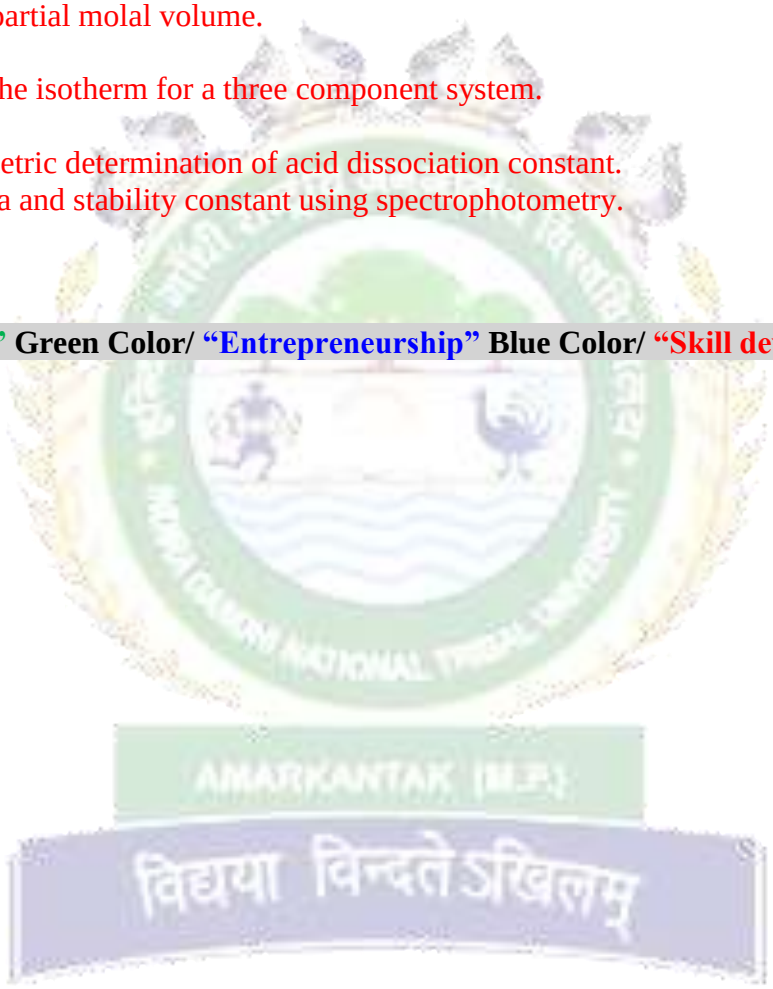

PAPER CODE: CHM P 422: ORGANIC CHEMISTRY PRACTICAL - II

SYLLABUS

Part A: Multi Step Synthesis of Organic Compounds

Multi step organic synthesis involving the concept of protecting groups and selectivity in organic reaction. A Student must be involved to check TLC for monitoring the reaction progress and doing column chromatography for purification.

Characterization of synthesized organic compoundsusing IR, UV and NMR, and mass spectroscopic techniques are to be studied.

- Nitrobenzene→aniline→Acetanilide (Nitration and followed by reduction)
- Malonic acid→cinnamic acid→methyl cinnamate (Condensation reaction and next followed by esterification)
- Benzaldehyde→benzoin→benzil→benzilic acid (Umpolung strategy, Oxidation reaction and next benzylic acid rearrangement reaction)
- Aniline→benzenediazonium chloride→benzeneazo-2-naphthol (Azodye synthesis)
- Skraup's synthesis: Quinoline from *o*-aminophenol (Heterocyclic compound synthesis)
- Acetanilide→p-acetamidobenzenesulfonylchloride→p-acetamidobenzenesulfonamide→sulfanilamide (Sulfa Drug synthesis)
- cinnamaldehyde→cinnamyl alcohol→cinnamyl bromide→allyl-aryl ether synthesis (Nucleophilic substitution reaction)

Part B: Extraction Method

- **Natural product extraction:** Solasidine, Caffeine, Nicotine, Peptine, Rosine, Carotenoids, Computational methods of retro-synthetic analysis modeling and calculation.

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SEMESTER – III

PAPER CODE: CHM T 511: PHYSICAL CHEMISTRY-III

(Chemical Bonding, Non-equilibrium Thermodynamics and Solid State Chemistry)

SYLLABUS

Unit – 1: Molecular Structure

Chemical bonding in diatomic; elementary concepts of MO and VB theories; Born-Oppenheimer approximation, MO treatment for H_2^+ ion, MO treatment of homo- and hetero- nuclear diatomic molecules; comparison of MO and VB theories. Hückel MO theory for conjugated π-systems. Polyatomic molecules, hybridisation and valence MOs of simple molecule like H_2O, NH_3, CH_4, C_2H_6 *etc*.

Unit – 2*: Ab-initio* Methods for Closed Shell Systems

Introductory treatment of semi-empirical and *ab-initio* calculations on molecular systems; the Hartree-Fock Self-Consistent Field Method; the generation of optimized orbitals, Koopman's theorem (The Physical Significance of Orbital Energies), electron correlation energy; density matrix analysis of the Hartree-Fock approximation, natural orbitals, matrix solution of the Hartree-Fock equations (Roothaan's equations); Hellman-Feynman theorem.

Unit – 3: Thermodynamics

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential, and entropies. Thermodynamics of open systems: partial molal properties, partial molal free energy, partial molal volume and partial molal heat content and their significances. Determination of these quantities. Concept of fugacity and determination of fugacity.
Non-ideal system: excess function for non ideal solutions. Activity, activity coefficient, Debye-Hückel theory for activity coefficient of electrolytic solution; determination of activity and activity coefficients; ionic strength.

Unit – 4: Non-equilibrium Thermodynamics

Thermodynamic criteria for non-equilibrium state, entropy production and entropy flow, energy balance equation for different irreversible processes (e.g. heat flow, chemical reaction etc.), transformation of the generalized fluxes and forces, non equilibrium stationary states, phenomenological equation, microscopic, reversibility and Onsager's reciprocity relations, electrokinetic phenomena, diffusion, electric conduction, irreversible thermodynamics for biological system, coupled reactions.

Unit – 5: Solid State Chemistry

Perfect and imperfect crystals, intrinsic and extrinsic defect, point defect, line and plane defect, vacancies, Schottky and Frankel defects; thermodynamics of Schottky and Frankel defect formation, color center, non-stochiometry defects. Metal insulators and semiconductors, electronic structure of solids-band theory, band structure of metals, insulators and semi-conductors, doping semi-conductors, *p-n* junction; superconductors; photoelectric effects; magnetic properties. Behaviour of substances in a magnetic field,

effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

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PAPER CODE: CHM T 512: INORGANIC CHEMISTRY –III

(Bio-Inorganic & Nuclear Chemistry)

SYLLABUS

Unit – 1: Bio-inorganic Chemistry – I

Transport and storage of dioxygen: Active site structures and bio functions of O_2-uptake proteins: hemoglobin, myoglobin, hemocyanin and hemerythrin; model synthetic dioxygen complexes. Chelato theraphy. Electron transfer in biology: Active site structures and functions of cytochromes, cytochrome *c*; iron-sulfur proteins (rubredoxin, ferredoxines), organic-redox protein cofactors – FAD, NAD, FMN, ubiquinone; blue copper proteins, HIPIP. Respiratory electron transport chain, cytochrome c oxidase. Photosynthesis and chlorophylls, photosystem-I and photosystem-II and their roles in cleavage of water. Model systems. Biological and abiological nitrogen fixing systems, model study.

Unit – 2: Advanced Bio-inorganic Chemistry – II

Metal ion interactions with purine and pyrimidine bases, nucleosides, nucleotides and nucleic acids, DNA and RNA, metal ions in genetic information transfer.

Redox enzymes: Catalase, peroxidase, super oxide dismutase (SOD), cytochrome P-450,

Nitrogen cycle enzymes: NO*x* reductases, nitric oxide synthases (NOS), ascorbate oxidase, aldehyde oxidase, sulfite oxidase, xanthine oxidase, nitrogenase, P and M clusters in nitrogenase, transition metal dinitrogen complexes and insights into N_2 binding, reduction to ammonia.

Unit – 3: Enzymes

Zinc enzymes, magnesium enzymes, iron enzymes, carbonic anhydrase, xanthine oxidase, aldehyde oxidase, cobalt containing enzymes, Mo and tungsten enzymes, Vitamin B-12
***Zinc in Transcription*:** Zinc fingers, zinc thiolate clusters.
***Calcium Signaling Protein*:** Calmodulin protein and Ca^{2+} ion pump
***Biological Cycle*:** Nitrogen cycle, hydrogen cycle, in vivo and vitro nitrogen fixation
***Sensors*:** Iron protein as sensor, Copper sensor, protein that sense copper and zinc level
***Other Application*:** Biominiralization, cancer treatment, antiarthristis drugs
Contribution of Individual Elements in Biological Function: Na, K, Li, Mg, Ca, Se, Mn, Fe, Co, Ni, Cu, Zn, Mo, W, Si, Pt, Au

Unit – 4: Inorganic Photochemistry

Introduction to inorganic photochemistry, photophysical and photochemical process. Excitation modes in transition metal complexes, fate of photo-excited species, fluorescence and phosphorescence applied to Inorganic systems, intramolecular energy transfer, vibrational relaxation, internal conversion and intrasystem crossing, quantum yield, decay fluorescence. Fluorence quenching, Stern-Volmer equation. Photochemical process: photo substitution and photoelectron transfer reactions in Co, Cr, Ru and Rh complexes.

Unit – 5: Nuclear Chemistry & Radiochemical Analysis

Nuclear models: **N**uclear stability, terrestrial abundance and distribution, relativistic effect, electronic

configuration, oxidation states, aqueous-, redox- and complex- chemistry; Nuclear forces, liquid drop model, shell model, Fermi gas model; magic numbers, nuclear spin and nuclear isomerism. *Nuclear reactions:* Energetics, mechanism and models of nuclear reactions. Nuclear fission and nuclear fusion, fission products and fission yields. Interactions of radiation with matters, chemical effects of nuclear transmutation (elementary idea), Nuclear reactors and particle accelerators.

Radioactive Techniques: Detection and measurement of radiation- GM ionization and proportional counters. Study of chemical reactions by tracer techniques, isotope exchange and kinetic isotope effect. Radiometric analysis: Isotope dilution analysis, age determination, neutron activation analysis (NAA) and their applications. Radiation hazards and safety measures.

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PAPER CODE: CHM T 513: ORGANIC CHEMISTRY –III

(Pericyclic Reaction, Photochemistry and Free Radical Chemistry)

SYLLABUS

Unit – 1: Introduction of Pericyclic Reaction

Definition, Symmetry of π molecular orbital, Filling of electrons in π molecular orbital in conjugated polyenes, conjugated ions, Frontier Molecular Orbital Theory, Classification of Pericyclic reactions

Unit – 2: Electrocyclic and Cycloaddition Reactions

***Electrocyclic Reactions*:** Conrotatory and disrotatory motion in ring opening and ring closing reactions, Frontier Molecular Orbital (FMO) approach for Electrocyclic reactions, Correlation diagram of the Electrocyclic reactions with 4nπ and (4n + 2)π electronic systems, Woodward – Hoffmann rule for Electrocyclic system.

***Cycloaddition Reactions*:** Theory of Cycloaddition reaction, Stereochemistry of Cycloaddition reaction, Diels-Alder reaction, 1, 3-Dipolar Cycloaddition reactions, Chelotropic reactions. Woodward – Hoffmann selection rule for Electrocyclic system.

Unit – 3: Sigmatropic Rearrangement and Group Transfer Reactions

Definition, Classification of Sigmatropic Rearrangement, Mechanism of Sigmatropic Rearrangement, Various types of [m, n] Sigmatropic rearrangements, Cope, Oxy-Cope and Claisen Rearrangement. Ene Reactions and Group Transfer Reactions given by Diimide.

Unit – 4: Photochemistry

***Basic Principle of Photochemistry and Reaction with Carbonyl compounds*:** Introduction of Photochemistry-Jablonski Diagram, Quantum Yield calculation of photo chemical reaction, photosensitizer and quencher; α-cleavage (Norrish type I & II) and β-cleavage reactions with carbonyl compounds, Intra- and Intermolecular Hydrogen abstraction reactions with carbonyl compounds, Photocycloaddition reactions (Paterno-Bűchi Reaction).

***Photo Rearrangement, Photo Reduction, and Photo Isomerization Reactions*:** Di- π-Methane Rearrangement, Aza-di- π-Methane Rearrangement, Photo reduction of carbonyl compounds, Cis-Trans Isomerization reactions with alkenes, Photochemistry of Dienes.

Unit – 5: Free Radical Reactions

Principles, Generation of free radicals, Formation of Carbon-Halogen bonds (Hundsdiecker reaction), Formation of Carbon-Carbon bonds (addition to carbon-carbon double bonds, Acyloin condensation reaction, Eglinton reaction). Formation of Carbon-Nitrogen bonds (Barton Recation and Hoffmann-Loeffler-Freytag Reaction).

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PAPER CODE: CHM P 511: PHYSICAL CHEMISTRY PRACTICAL – II

SYLLABUS

(i) Conductometry

(a) The measurement of electrical conductance for the determination of the equivalent conductance at infinite dilution.
(b) Determination of the activity coefficient of zinc ions in the solution of 0.002 M zinc sulfate using Debye-Hückel's limiting law.
(c) To verify Debye-Hückel limiting law for strong electrolyte.

(ii) (a) Rate of the hydrolysis of sucrose using polarimeter.
(b) Polarizability from refractive index measurement.

(iii) Potentiometry/pHmetry
(a) Determination of pKa of poly-basic acid with the pH meter.
(b) To determine the pH of various mixtures of acetic acid and sodium acetate in aqueous solutions and hence determine the dissociation constant of the acid.

(iv) Determination of the transport number by moving boundary method.

(v) IR and Raman spectroscopy of the solvent mixture.

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PAPER CODE: CHM P 512: INORGANIC CHEMISTRY PRACTICAL – II

SYLLABUS

I. Analytical Chemistry:

- Analysis of Ores: Felspar , bauxite, Rocks available in that region.
- Analysis of Soil sample, animal feeds, soil micronutrients, milk powder for Ca, Fe and P content.
- Separation of Mixture: Chromium (III) and Mn(II) in a mixture, Iron (III) and Cu(II) in a mixture, Iron(III) and Al(III) in a mixture

  At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session.

II. Preparations of Complex (At Least eight samples)

Preparation of selected inorganic compound and their studies by I.R. electronic spectra, Mössbauer and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds

1. bis(ethylene)nickel(II)thiosulphate,
2. tris(acetylacetonato)manganese(III), tris(acetylacetonato)Aluminium(III), tris(acetylacetonato)iron(II), tris(acetylacetonato)copper(II),
3. Hexaminecobalt(III)chloride,
4. Mercury tetrathiocyanatocobaltate(II),
5. Copper(II) biguanide
6. Mn_{12} Acetate Single Molecule Magnet
7. Preparation of copper glycine complex- cis and trans bis- (glycinato) copper (II).
8. Preparation of N, N-bis-(salicyldehyde) ethylenediamine, Co(salen), Mn(salen), determination of O_2 absorption by Co(salen), reaction of oxygen adduct with $CHCl_3$ (deoxygenation).
9. VO(*acac*)$_2$
10. *cis*-K $[Cr(C_2O_4)_2 (H_2O)_2]$
11. $Na[Cr(NH_3)_2 (SCN)_4]$
12. $K_2[Fe(C_2O_4)_3]$

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SEMESTER – IV

PAPER CODE: CHM T 521: MOLECULAR SPECTROSCOPY

SYLLABUS

Unit – 1: Unifying Principles

Electromagnetic radiation, interaction of electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarization, and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment selection rules, intensity of spectral line. Born-Oppenheimer approximation, rotational, vibrational, and electronic energy levels. Fourier Transform Spectroscopy.

Unit – 2: Microwave Spectroscopy

***Rotational spectroscopy*:** Classification of molecules, rigid rotor model, selection rule, intensity of spectral line, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect nuclear and electron spin interaction and effect of external field. Applications (determination of bond lengths of diatomic and linear triatomic molecules *etc*.)

Unit – 3: Vibrational Spectroscopy

A. *Infrared Spectroscopy*: Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strength; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P, Q, R branches. Breakdown of Oppenheimer approximation; vibration of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factor affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis. Fourier Transform Infra-red Spectroscopy (FTIR)

B. *Raman Spectroscopy*: Classical and quantum theories of Raman Effect, pure rotational, vibrational, and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti-stokes Raman spectroscopy (CARS).

Unit – 4: Electronic Spectroscopy

A. *Atomic Spectroscopy*: Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

B. *Molecular Spectroscopy*: Energy levels, molecular orbitals, vibranic transition, vibrational progressions and geometry of excited state, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complex, charge transfer spectra.

C. *Photoelectron Spectroscopy*: Basic principle; photo-electronic effect, ionization process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA, basic idea Auger electron spectroscopy.

Unit – 5: Magnetic Resonance, Photoacoustic, and Mössbauer Spectroscopy

A. *Nuclear Magnetic Resonance Spectroscopy*: Nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift and its measurement, factor influencing chemical shift, deshielding, spin-spin interaction, factor influencing coupling constant 'J'. Classification (ABX, AMX, ABC, A2B2 etc), spin decoupling; basic idea about instrument, NMR studies of nuclei other than proton – 13C, 19F, and 31P; FT NMR, advantage of FT NMR, use of NMR in medical diagnostics.

B. *Electron Spin Resonance Spectroscopy*: Basic principles, zero field splitting and Kramer's degeneracy, factors affecting the 'g' value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densityies and McConnell relationship, measurement techniques, applications.

C. *Nuclear Quadrupole Resonance Spectroscopy*: Quatrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting, applications.

D. *Photoacoustic Spectroscopy*: Basic principles of photoacoustic spectroscopy (PAS). PAS-gases and condensed system, chemical and surface applications.

E. *Mössbauer Spectroscopy*: Basic principles, spectral parameters and spectrum display. Application of technique to the studies of (i) bonding and structure of Fe^{2+} and Fe^{3+} compounds – nature of M-L bond, coordination number, structure and (ii) detection of oxidation state and inequivalent MB atom.

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PAPER CODE: CHM P 522: PROJECT AND DISSERTATION

Each student is assigned to a faculty supervisor to carry out a research project. They will be trained in searching research literature as well as experimental and computational work specific to the chosen research problem. On the basis of partial fulfilment of project report the student may go other University/Institute for project work. At the end of the project they will submit a report of the work done and make a presentation for evaluations.

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LIST OF ELECTIVE PAPER

S. No.	Course Code	Course Structure	Title of Paper	Credit
1	CHM T 601	Elective	Mathematics for Chemist	4
2	CHM T 602	Elective	Biology for Chemist	4
3	CHM T 603	Elective	Industrial Chemistry	4
4	CHM T 604	Elective	Instrumental Methods of Analysis	4
5	CHM T 605	Elective	Basic of Materials Chemistry	4
6	CHM T 606	Elective	Introduction to Nanomaterials and Nanotechnology	4
7	CHM T 607	Elective	Polymers Chemistry	4
8	CHM T 608	Elective	Bioorganic and Drug Chemistry	4
9	CHM T 609	Elective	Advanced Heterocyclic Chemistry	4
10	CHM T 610	Elective	Chemistry of Natural Products	4
12	CHM T 611	Elective	Solid State Chemistry	4
13	CHM T 612	Elective	Advanced Synthetic Organic Chemistry	4

PAPER CODE: CHM T 601: MATHEMATICS FOR CHEMIST (ELECTIVE)

SYLLABUS

Unit – 1: Vectors and Matrix Algebra

***Numbers*:** Real and Complex number
***Vectors*:** Vectors, dot, cross and triple product etc. The gradient, divergence and curl. Vector calculus, Gauss' theorem, divergence theorem *etc*.

Unit – 2: *Matrix Algebra*
Addition and multiplication; inverse, adjoint and transpose of matrices, special matrices (symmetric, screw-symmetric, Hermitian, screw-Hermitian, unit, diagonal, unitary etc.) and their properties. Matrix equations; homogeneous, non-homogeneous linear equation and conditions for the solution, linear dependence and independence. Introduction of vector spaces, matrix eigenvalues and eigenvectors, digonalization, determinants (examples from Hückel theory). Introduction to tensors; poarizability and magnetic susceptibility as examples.

Unit – 3: Differential and Calculus

Differential: Functions, continuity and differentiability, rules for differentiation, application of differential calculus including maxima and minima (examples related to maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell's distribution etc.), exact and inexact differentials with their application to the thermodynamic properties.

Partial Differential: Function of several variables, partial differentiation, co-ordinate transformation (e.g. Cartesian to spherical polar).
Integral calculus: basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus.

Unit – 4: Elementary Differential Equations
Ordinary first- and second-order differential equations. Partial differential equations. Solution of inexact differential equations by the method of integrating factors. Power series and extended power series solutions. Numerical solutions. Special functions: Hermite, Legendre and Laguerre polynomials, recursion relations.

Unit – 5: Probability and Curve Sketching
Permutation & Combination. Probability. Stirling's approximation. Lagrange multipliers. Curve sketching and curve fitting; Introduction to Fourier series and Fourier transforms.

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PAPER CODE: CHM T 602: BIOLOGY FOR CHEMIST (ELECTIVE)

(Biology for Chemist)

SYLLABUS

Unit – 1: Cell Structure & Functions

Structure of prokaryotic and eukaryotic cells, intracellular organelles and their function, comparison of plant and animal cells. Overview of metabolic processes-catabolism and anabolism; ATP the biological energy currency. Origin of life – unique property of carbon, chemical evolution and rise of living systems. Introduction to biomolecules, building blocks of bio-molecules.

Unit – 2: Carbohydrates

Conformation of monosaccharides, structure and function of important derivatives of monosaccharides like glycosides, deoxy sugars, myoinsitol, amino sugars, N-acetylmuramic acid, sialic acid, disaccharides and polysaccharides. Structural polysaccharides – cellulose, and chitin; storage polysaccharides – starch and glycogen. Structure and biological functions of glucosaminoglycans or mucopolysaccharides. Carbohydrates of glycoproteins glycolipids. Role of sugar in biological recognition. Blood group substances. Ascorbic acid, carbohydrate metabolism – Krebs' cycle, glycolysis, glycogenesis and glycogenolysis, gluconeogenesis pentose phosphate pathway.

Unit – 3: Lipids

Fatty acids, essential fatty acids, structure and function of triglycerols; glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins – composition and function, role in atherosclerosis. Properties of lipids, aggregates – micelles, bilayers, liposomes and their possible biological function. Biological membranes, fluid mosaic model of membranes structure. Lipid metabolism □-oxidation of fatty acids.

Unit – 4: Amino Acids

***Amino Acids, Peptides and Proteins*:** Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing, secondary structure of proteins, force responsible for holding of secondary structure. □-helix, □-sheet, super secondary structure, triple helix structure of collagen. Tertiary structure of proteins, folding and domain structure. Quaternary structure. Amino acid metabolism, degradation and biosynthesis of amino acids, sequence determination, chemical/enzymatic/mass spectral racemization detection. Chemistry of oxytocin and tryptophan releasing hormone (TRH).

Unit – 5: Nucleic Acids

Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids. The chemical basis of heredity, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono- and tri- nucleosides.

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PAPER CODE: CHM T 603: INDUSTRIAL CHEMISTRY (ELECTIVE)

SYLLABUS

Unit – 1: Water and Its Treatment

Sources of water, chlorinated and nonchlorinated water, chemical method of sterilization: precipitation method, Aeration, ozonisation, chlorination, chloramines process, potassium permanganate method, Physical method of sterilization: Boiling, exposure to sunlight, hard and soft water, Types of hardness, temporary and permanent hardness, water softening, cold and hot lime soda process, zeolite process, ion exchange process, removal of iron, silica, and dissolved oxygen from water for industrial purposes, water for boiler uses, water analysis.

Unit – 2: Glass and Rubbers

***Glass*:** physical and chemical properties of glass, constituents in glasses, raw materials, manufacturing of glasses, optical glass, borosilicate glass, lead glass, colored glass, opal glass, safety glass, fiber glass.

***Natural and Synthetic Rubber*:** classification of rubber, natural and synthetic rubber.

Unit – 3: Chemical Fertilizers

Classification of fertilization, nitrogeneous fertilizers, method of production and its action- ammonium nitrate, ammonium sulphate, urea, calcium cyanamide, ammonium chloride, phosphate rock, normal super phosphate, triple super phosphate.

Unit – 4: Petroleum

Classification of petroleum, composition of petroleum, mining of petroleum, refining of petroleum, octane rating, octane number and antiknock compound, cetane number, production of gases, crude naptha, benzene, kerosene oil, fuel oil, lubricating oil, paraffin wax and black tarry after refining. Cracking: thermal cracking, hydrocracking, and fluid catalytic cracking.

Unit – 5: Fibers and Dyes

***Synthetic Fibers*:** Preparation of fibers- Nylons, Nylon-66, Nylon-6, Nylon-11, Nylon-610, Nylon-8, polyethylene terephthalate, orlon, saran, vinyon, taflon.

***Synthetic Dyes and Dyeing*:** Requisites of true dyes, sensation of color, witt's theory, chromophores, auxochromes: batho-, hypso-, hyper-, and hypochromic shifts; classification of dyes: acid dyes, basic dyes, adjective dyes, vat dyes, ingrain dyes, sulfur dyes, pigment dyes, nitroso dyes, nitro dyes, azo dyes, xanthenes dyes, applications of dye.

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PAPER CODE: CHM T 604: INSTRUMENTAL METHODS OF ANALYSIS (ELECTIVE)

SYLLABUS

Unit – 1: Molecular Spectroscopy

Nature of electromagnetic radiation, electromagnetic spectrum, atomic, molecular and vibrational energy levels, basic instrumentation- source of radiation, monochromator, sample cells, absorber, detector, UV-Vis detector, photomultiplier, IR detector, display and recorder, single and double beam spectrophotometer, Beer Lambert law, deviation from beers law, ultraviolet and visible spectroscopy, Fluorescence and phosphorescence spectrophotometer, Fourier transform infrared spectrometer and Raman spectrometer, instrumentation, techniques and application.

Unit – 2: Atomic Spectroscopy

Flame emission spectrometry, atomic absorption spectroscopy- principle, instrumentation, Source in AAS – Hollow cathode lamp, electrode less discharge lamp, burners, nature and property of flame, interference in AAS, difference between AAS and FES, ICP.

Unit – 3: Thermal Analysis

Types of thermal method, Thermogam, thermogravimetric analysis(TGA), differential thermal analysis(DTA), differential scanning calorimetry (DSC), schematic diagram for TGA and DTA instruments and their working principle, factors affecting thermogram like geometry of sample holder, furnace atmosphere, heating rate, particle size, packing of sample, weight of sample, analysis of metals or oxide in mixture, application of TGA and DTA.

Unit – 4: Chromatography

Principles of chromatographic separation, classification of Chromatographic Techniques: adsorption, partition, ion exchange and size exclusion chromatography, theory of chromatographic separation, distribution coefficient, retention time, sorption, theory of column efficiency and resolution, separation factor, retention factor. – working principle and application of Column chromatography, ion exchange chromatography, paper chromatography, Thin layer chromatography (TLC) & HPTLC: techniques and application. - Gas Chromatography and high performance liquid chromatography: Van Deemter equation, retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Unit – 5: Electroanalytical Techniques

Electrochemical cells, current potential relationship, mass transfer by migration, convection and diffusion, Electrogravimetry, voltam-metry, polarography, reference electrode, working electrode, auxiliary electrode, dropping mercury electrode, current potential curve, limiting current, coulometry, conductometry methods, instrumentation, techniques and application. Amperometric titration, effect of electroactive and reagent on amperometric curve and its advantage, rotating platinum electrode, biamperometric titration and its advantage, fluorimetry and phosphorimetry.

PAPER CODE: CHM T 605: BASIC OF MATERIALS CHEMISTRY (ELECTIVE)

SYLLABUS

Unit – 1: Chemical Crystallography

***Introduction*:** Space lattice, crystal point groups, space group (working knowledge), stereographic projections, packing in solids, crystal structures of representative systems, silicates and zeolites, cements, glasses, quasicrystals, nanostructures.

***Bonding in Solids and Crystal Energetics*:** Crystal classifications, Madelung constant and Lattice energy.

Unit – 2: Characterization Techniques for Solids

X-ray diffraction, electron microscopy (SEM, TEM, AFM), thermal techniques (TG, DTA, DSC), spectroscopic techniques (Mössbauer, IR, UV-VIS), and physical property measurement techniques (magnetic moments-VSM/SQUID, electrical resistivity – two / four probe methods and thermal conductivity, optical band gap, XPES, XAS.

Unit – 3: Electronic and Magnetic Properties Solids

Electronic Properties and Band Theory of Solids: Free electron theory of metals, Band theory of solids, Bloch theorem, Kroning-Penne model, refinement of simple band theory- *k*-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, *p*-*n* junctions.

***Magnetic Properties Solids*:** Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis. Introduction of superconductors, Meissner effects, basic concepts of BCH theory.

Unit – 4: Defects and Phase Transitions

***Defects, Nonstoichiometry and Diffusion*:** Point defects, dislocations, extended defects, clusters and aggregates, color centers, nonstoichiometry of compounds, diffusion mechanisms, Fick's law, Kirkenall effect.

***Phase Transitions*:** Critical phenomena, variety of phase transitions (ordered-disorder, Martensite-austenite, spinoidal decompositions *etc*), liquid crystals, structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

Unit – 5: Preparative Techniques

***Reactivity of Solids*:** Decomposition and reactivity, solid state reactions, sintering process, reaction kinetics, organic solid reactions.

***Conventional Techniques*:** Powder mixing, fusion, precipitation from solution, modern need for improved synthetic routes, crystal growth and thin film techniques.

Chemical Routes: Wet-chemical (Oxidation-reduction for metal nanoparticles) methods, self assembly

methods, reverse micelles route, biomimetic, sonochemical, and electrochemical approaches.

***Sol-Gel Synthesis*:** Colloids, cation hydrolysis and sol formation, gel precipitation, sol-gel process for colloids, synthesis andphysical properties of metal alkoxides, development of sol-gel process from alkoxides, derived coatings, fibers and monodispersed submicron/ nanostructured oxide powders, ormosils, sialons.
***Hydrothermal/Solvothermal Approach*:** Forced hydrolysis at elevated temperatures and pressures, hydrothermal reactions using salt solutions, metal reactants and reactions involving phase transformation.

***Precursor Technique*:** Citrate-gel process, metallo-organic precursors, metal alkoxides.

***Gas Phase Reactions*:** Gas-phase nucleation, flame hydrolyzed powders, direct - nitridation and carbothermic reduction, non-plasma gas phase reactions, plasma reactions, electron beam evaporation.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 606: INTRODUCTION TO NANOMATERIALS AND NANOTECHNOLOGY (ELECTIVE)

SYLLABUS

Unit – 1: Nanoscience and Nanotechnology

***Introduction*:** Underlying physical principles of nanotechnology: *Nanostructured Materials: Size is Everything*. Fundamental physicochemical principles, size and dimensionality effects; quantum confinement; properties dependent on density of states; single electron charging, central importance of nanoscale morphology. Societal aspects of nanotechnology: health, environment, hype and reality.

***Type of Nanostructures*:** Definition of a nano system; one dimensional (1D), two dimensional (2D), three dimensional (3D) nanostructured materials; quantum dots; quantum wire, and core/shell structures.

Unit -2: The Basic Tools of Nanotechnology

Electron microscopy (SEM, TEM with EDX analysis) and X-ray diffraction, A brief historical overview of atomic force microscopy (AFM); an introduction and basic principles & applications of XPS, FTIR spectrophotometers; UV-VIS principle and application for band gap measurement.

Unit – 3: Synthesis of Nanomateirals

Top down and bottom up approaches to synthesis of nanomaterils:

***Chemical Routes for Synthesis of Nanomaterials*:** Chemical precipitation and co-precipitation; sol-gel synthesis; microemulsions or reverse micelles; solvothermal synthesis; thermolysis routes, microwave heating synthesis biomimetic and electrochemical approaches; sonochemical synthesis; photochemical synthesis; synthesis in supercritical fluids.

***Physical Routes for Preparation of Nanomaterial*:** Inert gas condensation, arc discharge, RF plasma, plasma arc technique, ion sputtering, laser ablation, laser pyrolysis, spray pyrolysis, ball milling, molecular beam epitaxy, chemical vapour deposition method, Langmuir-Blodgett (LB) films, spin coating and electro deposition.

Unit – 4: Nanomateirals and Properties

Synthesis and size dependent properties (mechanical, physical and chemical properties) of carbon nanotubes (CNT); metals (Au, Ag); metal oxides (TiO_2, CeO_2, ZnO); semiconductors (Si, Ge, CdS, ZnSe); dilute magnetic semiconductor.

Unit -5: Applications of Nanomateirals

Basic ideas of nanodevices (molecular electronics and nanoelectronics, and quantum electronic devices); CNT based transistor and field emission display; biological applications; biochemical sensor; membrane based water purification, energy storage devices, catalysis and various related fields.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 607: POLYMERS CHEMISTRY (ELECTIVE)

SYLLABUS

Unit – 1: Introduction

Importance of polymers. Basic Concept: monomers, repeat units, degree of polymerization; linear, branched, and network polymers (block-copolymer, dendrimer etc.); classification of polymers. Polymerization: condensation, addition, radical, chain- ionic- and co-ordination-, and co-polymerization; polymerization condition and polymer reaction; polymerization in homogeneous and heterogeneous systems.

Unit– 2: Polymer Characterization Techniques

Polydispersion-average molecular weight concept; number, weight and viscosity average molecular weights. Polydiversity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group, viscosity, light scattering, osmotic, and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers. Spectroscopic methods, X-ray diffraction, microscopy studies. Thermal analysis and physical testing tensile strength, fatigue, impact, tear resistance, hardness and abrasion resistance analysis.

Unit – 3: Structure and Properties

Morphology and order in crystalline polymers – configuration of polymer chains; crystal structure of polymers; morphology of crystalline polymers; strain-induced morphology; crystallization and melting polymer structure and physical properties – crystalline melting point, T_m, melting points of homogeneous series effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g, relationship between T_m and T_g, effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Properties requirements for polymer utilization.

Unit – 4: Polymer Processing

Plastic, elastomers and fibres, compounding; processing techniques- calendaring, die casting, rotational casting, film casting, injection casting, blow moulding, extraction moulding, thermoforming, foaming, reinforcing, and fibre spinning.

Unit – 5: Properties of Commercial Polymers

Polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resins, epoxy resins and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 608: BIOORGANIC AND DRUG CHEMISTRY (ELECTIVE)

SYLLABUS

Unit – 1: Overview of Bioorganic Chemistry

***Introduction*:** Definition of bioorganic chemistry, Border line of bioorganic chemistry and inter disciplinary area between chemical and biology, Weak interaction in organic and biological world, Molecular Recognition.

***Chemistry of the Living Cell*:** The structure of prokaryotic and Eukaryotic cells, Composition of living cells:

Unit – 2: Carbohydrates, Proteins, Lipids, and Nucleic Acids

***Carbohydrates*:** Introduction, Reactions of Monosaccharides, Interconversions, Ring structure of aldoses and ketoses, Confirmation of Monosaccharides, Disaccharides: Structure, synthesis and properties.

***Proteins*:** General structure & classification of amino acids, Abbreviation of amino acids, Essential and non essential amino acids, Synthesis of amino acids, Isoelectric point, Acid and base properties of amino acids. Protein: Naturally occurring peptides, Modern methods of peptide synthesis with protection and deprotection, Determination of sequences and basic units of a poly peptides or proteins, C- & N-terminus detection by chemical methods, Primary, secondary, tertiary and quaternary structures of proteins, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases etc.

***Lipids*:** Lipid structure- acylglycerols, phosphoglycerides and sphingolipids, Biological importance of fatty acids and lipids, Bio- and chemical Synthesis of lipids.

***Nucleic Acids*:** Definition, structure and properties, base pairing, double helices, Genetic information storage, transmission and gene expression, Nucleotides and Nucleosides: Similarities and differentiation, Structure of DNA & RNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis.

Unit – 3: Analogy Between Biochemical and Organic reactions

Introduction to metabolism (catabolism, anabolism). ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD^+, FAD. Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle. Overview of catabolic pathways of fat and protein. Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types.

Unit – 4: Overview of Drug Chemistry and Basics of Drug Action

Definition, classification and nomenclature of drugs, Preliminary idea of drug action: Interaction (Weak interaction in drug molecules, Chirality and drug action), Receptorology (Drug-receptor interactions, Enzyme kinetics in drug action, Enzyme inhibitors (Drug action through enzyme inhibition), Nucleic acids as targets for drug actions, NA-Alkylation, NA-strand breaking and their importance in drug action, Drug metabolism, drug deactivation and elimination.

Unit – 5: Pharmaceutical Compounds: Structure and Importance

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 609: ADVANCED HETEROCYCLIC CHEMISTRY (ELECTIVE)

SYLLABUS

Unit – 1: Introduction

Definition of heteroatom, Aromatic and non-aromatic heterocyclic compounds, Classification and nomenclature of heterocyclic compounds, important reactions with heterocyclic compounds i.e. oxidation, reduction and tertiary effect of Nitrogen in heterocyclic compound.

Unit – 2: Non-Aromatic Heterocycles

Different types of strains, interactions and conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of the following ring systems: Aziridines, Oxiranes, Thiiranes, Oxaziridines, Azetidines, Oxetanes and Thietanes.

Unit – 3: Five and Six Membered Heterocyclics with One Hetero Atom

Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions [Advanced synthetic methods are applied].

Unit – 4: Five and Six Membered Heterocyclics with Two Hetero Atoms

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

Unit – 5: Larger Ring and Other Heterocycles

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Benzoazepines, Benzooxepines, Benzothiepines, Azocines and Azonines.

"Employability" Green Color/ "Entrepreneurship" Blue Color/ "Skill development" Red Color

PAPER CODE: CHM T 610: CHEMISTRY OF NATURAL PRODUCTS (ELECTIVE)

SYLLABUS

Unit – 1: Alkaloid – I

Occurrence and isolation, biological role of alkaloids, General properties, nomenclature and classification of alkaloids on the basis of amino acid origin and present core structure. Isolation, properties and structural elucidation of quinine, Morphine (structure, synthesis, molecular rearrangement, stereochemistry and biogenesis).

Unit – 2: Alkaloid – II

Structure and biological role of nicotine, cocaine, quinine, reserpine, vincristine, morphine, caffeine, papavarine, hyocimine. Strychnine and lysergic acid.

Unit – 3: Steroid

Introduction, nomenclature of steroids, absolute configuration of steroid. Occurrence, isolation, structute elucidation and chemical properties of Cholesterol.

Unit – 4: Terpenes

Secondary metabolites: Definition and examples; terpenes – isoprene rule; mono terpenes: structure of geraneol, limonene, alpha-pinene and camphor; sesquiterpenes: longfolene;

diterpenes: abietic acid, taxol. Structure determination of Citral and Camphor.

Unit – 5: Vitamins

Introduction, chemical properties, structure elucidation of Vitamin A, Vitamin B, Ascorbic Acid and Vitamin D. Vitamin A and its role in vision. Biological role of Vitamin D, Ascorbic Acid, Vitamin A.

PAPER CODE: CHM T 611: SOLID STATE CHEMISTRY (ELECTIVE)

SYLLABUS

Unit – 1: Crystal Structure

Crystalline and amorphous solids; symmetry in crystals, basic crystal systems,space lattice and unit cell, Bravais lattice,miller indices, closed packed structure- hcp and ccp, packing efficiency, limiting radius ratio and shape of ionic crystal, description of solids; structure types Rock salt (NaCl), Zinc blende (ZnS),antifluorite(Na_2O), Rutile (TiO_2), Wurzite (ZnS), $CdCl_2$, nickel arsenide, CsCl, CdI2, Cs_2O, perovskite ABO_3, K_2NiF_4, spinels.

Unit – 2: Point Groups

Symmetry operation and symmetry elements, Plane of symmetry, inversion centre, proper and improper axis of rotation, Product of symmetry operation, Relation among symmetry elements and symmetry operation, classification of symmetry, symmetry elements in octahedral and tetrahedral molecules, symmetry point group, representation of symmetry operation by matrices, reducible and irreducible representation, Character tables.

Unit – 3: Space Groups

Thirty two point groups, Representation of point groups and selected examples like 222, mm2, mmm, 32 centrosymmetric and noncentrosymmetric point groups, space group: Triclinic P1, monoclinic C2, monoclinic C2/m, orthorhombic $P222_1$ orthorhombic F222, Tetragonal 14_1 , space group and crystal structure of $SrTiO_3$ and rutile structure of TiO_2.

Unit – 4: Structure and Properties of Advance Materials – I

Superconductors – (Ba,K)BiO_3, Cuprates, LnFeAsO, MgB_2, CaC_6
CMR materials – $La_{(1-x)}Sr_xMnO_3$
Ferroic compounds – $BaTiO_3$, $PbTiO_3$, $Bi_4Ti_3O_{12}$, $SrRuO_3$
Peizoelectric materials- PZT,
Photoluminescent materials – Lanthanide compounds
Porous materials – zeolites, AlPO, MeAlPO, SAPO.

Unit – 5: Structure and Properties of Advance Materials – II

Organic-inorganic hybrid materials – MOF compounds
Ionic Conductors – NASICON, AgI, $NaAl_{11}O_{17}$
Thermoelectric materials – $NaxCoO_2$, $AgSbTe_2$, $CoSb_3$, $Y_{14}MnSb_{11}$
Compounds for intercalation and redox reactions – $LiCoO_2$, $LiVS_2$, NASICON, Chevrel phases

PAPER CODE: CHM T 612: ADVANCED SYNTHETIC ORGANIC CHEMISTRY (ELECTIVE)

SYLLABUS

Unit – 1: Metal Mediated C-C and C-X Coupling Reactions

Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia Lythgoe olefination and Peterson's stereoselective olefination. Olefin metathesis by Ist and IInd generation catalysts: Reaction mechanism and application in the synthesis of heterocycles.

Unit– 2: Reagents of Phosphorous, Sulfur, Silicon and Boron

Phosphorous Sulfur, Silicon and Boron containing compounds-preparations and their uses in organic reactions.

Unit – 3: Oxidation and Reduction

***Oxidation*:** Oxidation of hydrocarbons (alkanes, aromatic hydrocarbons, alkenes), Oxidation of alcohols (Chromium reagents, Manganese reagents, Other metal and non-metal based oxidants), Oxidation of ketones (α, β-unsaturated ketones, α-hydroxy ketones, Baeyer-Villiger oxidation of ketone)

***Reduction*:** Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents (Derivatives of lithium aluminium hydride and sodiumborohydride, mixed lithium aluminium hydride-aluminium chloride reagent, DIBAL-H, $NaBH_3CN$, sodium triacetoxyborohydride, Borane and derivatives, other methods of reductions).

Unit – 4: Disconnection Approach, Umpolung Chemistry and Protection-Deprotection of Functional groups

Basic principles and terminology-Target molecule, FGI, Disconnection, Synthon, Reagent and Retro-synthetic approach. **One group C-C and C-X disconnection**: (disconnection of alcohols, alkenes, and carbonyl compounds). **Two group C-C & C-X disconnections**: 1,3 and 1,5 difunctionalised compounds, α, β, unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels- Alder reaction, connection in retro synthesis. Umpolung in organic synthesis. Protection and deprotection for functional groups as hydroxyl, amino, carboxylic and carbonyl.

Unit – 5: Some Important Organic Reactions

Selective Stereoselective Organic Reactions with Alkenes: Sharpless Asymmetric Epoxidation, Asymmetric Aziridination, Dihydroxylation, Amino-hydroxylation Reactions, Oxidative cleavages of alkenes.

Green Chemistry, Supramolecular chemistry (Crown ether, Cyclodextrin and Clalixerins) and multicomponent reactions (Ugi, Passerini, Biginelli, Hantzsch reactions).

***Chemistry of Aliphatic and Aromatic Heterocyclic Compounds*:** Epoxide, Aziridine, Azitidine, Oxetane, Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions.