COURSES OF STUDIES

FOR POST GRADUATE DEGREE
IN CHEMISTRY
(SEMESTER SYSTEM)

Session: 2021-22

GANGADHAR MEHER UNIVERSITY,
AMRUTA VIHAR, SAMBALPUR-768004

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 recognised centre for chemical sciences and to establish state of art centralise 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 andenvironment.

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

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

PROGRAM ARTICULATION MATRIX

SEMESTER	COURSE CODE	PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
I	CHE 101	3	2	1	2	1	2	2	2	2	0	3
	CHE 102	2	2	2	1	0	1	2	2	1	0	2
	CHE 103	2	2	0	1	0	1	1	2	1	2	2
	CHE 104	3	2	2	1	1	2	0	3	2	0	3
	CHE 105	3	0	1	3	1	3	3	3	3	3	3
II	CHE 201	3	2	1	2	1	3	2	3	2	3	3
	CHE 202	3	2	3	1	1	2	2	3	1	0	2
	CHE 203	3	2	0	3	0	2	1	3	3	3	3
	CHE 204	3	2	0	1	0	2	3	3	2	0	3
	CHE 205	3	0	2	2	2	0	0	1	3	3	1
	CHE 206	2	2	0	1	2	1	2	2	0	0	2
III	CHE 301	3	2	1	3	1	2	3	3	0	2	3
	CHE 302	3	2	2	1	2	3	3	3	0	0	3
	CHE 303	2	2	0	1	0	1	2	2	1	2	2
	CHE 304	3	2	0	0	0	2	3	3	2	0	3
	CHE 305	3	0	2	1	2	2	3	3	2	3	3
	CHE 306	2	1	1	3	2	1	3	3	2	0	3
IV	CHE 401	3	2	1	1	1	2	3	1	1	0	3
	CHE 402	3	2	2	3	2	2	3	2	2	0	3
	CHE 403	3	2	0	0	0	2	2	1	0	0	3
	CHE 404	3	1	0	0	0	3	1	2	0	3	3
	CHE 405	3	1	0	1	2	2	2	1	3	3	3
AVERAGE		2.77	1.59	0.95	1.54	0.95	1.86	2.0	2.31	1.5	1.22	2.68

M.Sc. Chemistry 2021-22

Year	FIRST SEMESTER						SECOND SEMESTER					
	Course Code	Course Name	L	T	P	C	Course Code	Course Name	L	T	P	C
I	CHE 101	Inorganic Chemistry I	3	1	0	4	CHE 201	Inorganic Chemistry II	3	1	0	4
	CHE 102	Organic Chemistry I	3	1	0	4	CHE 202	Organic Chemistry II	3	1	0	4
	CHE 103	Physical Chemistry I	3	1	0	4	CHE 203	Physical chemistry II	3	1	0	4
	CHE 104	Organic spectroscopy	3	1	0	4	CHE 204	Bioinorganic and Supramolecular Chemistry	3	1	0	4
	CHE 105	Inorganic Practical	0	0	12	4	CHE 205	Organic Practical	0	0	12	4
							CHE 206	**DSE (A/ B/ C)	3	1	0	4
			12	4	12	**20**			15	5	12	**24**
	Total Contact Hours (L + T + P)		**28**				**Total Contact Hours (L + T + P)**		**32**			
II	**THIRD SEMESTER**						**FOURTH SEMESTER**					
	CHE 301	Inorganic Chemistry III	3	1	0	4	CHE 401	Inorganic Chemistry IV	3	1	0	4
	CHE 302	Organic Chemistry III	3	1	0	4	CHE 402	Organic Chemistry IV	3	1	0	4
	CHE 303	Molecular Spectroscopy	3	1	0	4	CHE 403	Physical Chemistry III	3	1	0	4
	CHE 304	Material chemistry	3	1	0	4	CHE 404	Physical Chemistry IV	3	1	0	4
	CHE 305	Physical Practical	0	0	12	4	CHE 405	Project	0	0	12	4
	CHE 306	**IDSE (A/ B/ C)	3	1	0	4						
			15	5	12	**24**			12	4	12	**20**
	Total Contact Hours (L + T + P)		**32**				**Total Contact Hours (L + T + P)**		**28**			

22 PAPERS × 100 marks each	Grand Total marks = 2200	**Total credits: 88**

**** DISCIPLINE SPECIFIC ELECTIVE (DSE)**

DSE: CHE 206 [Group (A/ B/ C)]	**IDSE: CHE 306 [Group (A/ B/ C)]**
1. A: Analytical Chemistry 2. B: Surface Chemistry and Catalysis 3. C: Computational Chemistry and Molecular Modelling	1. A: Environmental Chemistry 2. B: Industrial Process 3. C: Matter and Energy Balance

DSE: Discipline specific elective (opted by students of the department. Minimum student strength to run the any course = 8)
IDSE: Inter Discipline specific elective (opted by students of the other department.)

POST GRADUATE PROGRAMME STRUCTURE
SCHOOL 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			
CHE 101 (THEORY)	INORGANIC CHEMISTRY I	80	20	100	3	4
CHE 102 (THEORY)	ORGANIC CHEMISTRY I	80	20	100	3	4
CHE 103 (THEORY)	PHYSICAL CHEMISTRY I	80	20	100	3	4
CHE 104 (THEORY)	ORGANIC SPECTROSCOPY	80	20	100	3	4
CHE 105 (PRACTICAL)	INORGANIC PRACTICAL	80	20	100	3	4
Total				500		20

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			
CHE 201 (THEORY)	INORGANIC CHEMISTRY II	80	20	100	3	4
CHE 202 (THEORY)	ORGANIC CHEMISTRY II	80	20	100	3	4
CHE 203 (THEORY)	PHYSICAL CHEMISTRY II	80	20	100	3	4
CHE 204 (THEORY)	BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY	80	20	100	3	4
CHE 205 (PRACTICAL)	ORGANIC PRACTICAL	80	20	100	3	4
DSE PAPERS CHE 206A CHE 206B CHE 206C	A. ANALYTICAL CHEMISTRY B. SURFACE CHEMISTRY AND CATALYSIS C. COMPUTATIONAL CHEMISTRY & MOLECULAR MODELLING	80	20	100	3	4
Total				600		24

*Discipline specific elective paper: Any paper can be opted by students of the department. Minimum student strength to run the course in elective paper should be 8.

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			
CHE 301 (THEORY)	INORGANIC CHEMISTRY III	80	20	100	3	4
CHE 302 (THEORY)	ORGANIC CHEMISTRY III	80	20	100	3	4
CHE 303 (THEORY)	MOLECULAR SPECTROSCOPY	80	20	100	3	4
CHE 304 (THEORY)	MATERIAL CHEMISTRY	80	20	100	3	4
CHE 305 (PRACTICAL)	PHYSICAL PRACTICAL	80	20	100	3	4
DSE PAPERS CHE 306A CHE 306B CHE 306C	A. ENVIRONMNETAL CHEMISTRY B. INDUSTRIAL PROCESS C. MATTER & ENERGY BALANCE	80	20	100	3	4
Total				600		24

*Inter Discipline specific elective paper: Any paper can be opted by students of the other department.

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			
CHE 401 (THEORY)	INORGANIC CHEMISTRY IV	80	20	100	3	4
CHE 402 (THEORY)	ORGANIC CHEMISTRY IV	80	20	100	3	4
CHE 403 (THEORY)	PHYSICAL CHEMISTRY III	80	20	100	3	4
CHE 404 (THEORY)	PHYSICAL CHEMISTRY IV	80	20	100	3	4
CHE 405 (PROJECT)	PROJECT WORK AND SEMINAR	100		100	3	3+1
Total				500		20
22 PAPERS	Grand Total	2200				88

*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 CHE 101: INORGANIC CHEMISTRY I

Full Mark 100 (80 + 20)

Course Objectives: The learners should be able to apply, analyze and evaluate the structure and bonding of main group and transition elements and their reaction properties and various structural features of compounds formed by these elements

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

[CHE101.1]. Recall basic properties of main group elements and understand various synthetic methods of important main group compounds.
[CHE101.2]. Recognize important applications of main group elements.
[CHE101.3]. Interpret magnetic properties of transition metal complexes.
[CHE101.4]. Examine their electronic spectra.
[CHE101.5]. Describe the basic properties of d-block and f-block elements.

B. SYLLABUS

UNIT 1 Chemistry of main group elements A: General characteristics, Structure and Reactions of simple and industrially important compounds: Boranes, Carboranes, Silicones, Silicates, Borazines and Phosphazenes.
UNIT 2 Chemistry of main group elements B: General characteristics, Structure and Reactions of simple and industrially important compounds: Hydrides, Oxides and Oxoacids of pnictogens (N, P), chalcogens (S, Se &Te) and halogens, Xenon compounds, Pseudo halogens and Interhalogen compounds.
UNIT 3 Transition elements: Coordination chemistry of Transition Metal ions, Stabilization of Unusual oxidation states, Stereochemistry of coordination compounds, splitting of d-orbitals in Low symmetry environment, Jahn-Teller effect, Interpretation of Electronic Spectra including Charge Transfer Spectra, Spectrochemical series, Nephelauxetic series, Fluxional molecules, Spinel & Inverse Spinel.
UNIT 4 **Inner transition elements:** Chemistry of Lanthanides and Actinides: Lanthanide Contraction, Separation of Lanthanide elements, Oxidation state, Spectral and Magnetic Properties, Stereochemistry, Use of LanthanideCompounds as Shift reagents, Actinide contraction, Oxidation states, Comparisons betweenLanthanides and Actinides.

C. TEXT BOOKS

1. Shriver D. E ,Atkins P. W., Inorganic Chemistry, Oxford University Pres ,5thEdn.
2. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4 th Ed. Harper Collins (1993)

D. BOOKS FOR REFERENCES

1. Advanced Inorganic Chemistry by F. A. Cotton and G. W. Wilkinson, John-Wiley & Sons, 1988, 5th Ed.
2. Chemistry of the Elements: N. N. B. Greenwood and A. Earnshow, Pergamon.
3. Comprehensive Coordination Chemistry G. Wilkinson, R. D. Gillars and J. A. McCleverty, Pergamon.
4. Das Asim K., Fundamentals of Inorganic Chemistry, Vol. II, CBS Publications, 2nd Ed. 2010.

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

CO	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	PSO3	PSO 4
CHE101.1	Recall basic properties of main group elements and understand various synthetic methods of important main group compounds.	3		2				2	2			2
CHE101.2	Recognize important applications of main group elements.	2	2				2		2	1		1
CHE101.3	Explain magnetic properties of transition metal complexes.	1			2		2				3	2
CHE101.4	Learn the properties of highly important transition metals in great details.	2		1			2			2	2	2
CHE101.5	Describe the basic properties of d-block and f-block elements.	2		1		3		2	2			3

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

PAPER CHE 102: ORGANIC CHEMISTRY I

Full Mark 100 (80 + 20)

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

[CHE 102.1]. Understand the mechanism, types of reactions and the factors affecting reactions
[CHE 102.2]. Learn about the aliphatic nucleophilic Substitution reaction and corresponding name reactions
[CHE 102.3]. Learn about the aromatic nucleophilic Substitution reaction and corresponding name reactions
[CHE 102.4]. Apply concepts associated with these general reaction types to product prediction.
[CHE 102.5]. Apply the concept of free radical reaction in predicting the product of the reaction

B. SYLLABUS

UNIT-1 : Reaction mechanism: Structure and reactivity

(a) Types of mechanism, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, isotope effects. (b) Organic reactive intermediates: methods of generation, structure, stability
and important reactions The Hammett equation and linear free energy relationships,Taft equation.

UNIT-2 : Aliphatic Nucleophilic and Electrophilic Substitution reactions.

(a) Aliphatic Nucleophilic Substitution reaction

The SN2, SN1, mixed SN1 and SN2 and SET mechanisms. The neighbouring group participation. Classical and nonclassical carbocations, phenonium ions, norbornyl system. Application of NMR spectroscopy in the detection of carbocations. Reactivity: effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis.

(b) Selective Organic name reactions:

Favorski reaction, Stock enamine reaction, Sharpless asymmetric epoxidation, Barton reaction, Chichibabin reaction, Claisen condensation, Dieckmann condensation, Horner-Wadsworth-Emmons olefination, Wittig olefination, Mitsunobu reaction, Fries rearrangement, Peterson olefination, McMurry Coupling

(c) Aliphatic Electrophilic Substitution reaction:

Bimolecular mechanisms (SE2) and SEi. Effect of substrates, leaving group and the solvent polarity on the reactivity.

UNIT-3 : Aromatic Nucleophilic and Electrophilic Substitution reactions.

(a) Aromatic Nucleophilic substitution: The SNAr, SN*i* benzyne and SRN1 mechanisms. Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements. (b) Aromatic Electrophilic substitution:
Areniun ion mechanism, orientation and reactivity. Diazonium coupling, Vilsmeier reaction, Gattermann- Koch reaction.

UNIT-4 : Free Radical Reaction.

Types of free radical reactions: Free radical substitution mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. The effect of solvents on reactivity. Allylic halogenation (NBS), free radical rearrangement, Hunsdiecker reaction.

C. TEXT BOOKS

1. Jonathan Clayden, Nick Greeves, Stuart Warren, Organic Chemistry, 2nd Edition, Oxford Publisher, 2014.

D. BOOKS FOR REFERENCES

1. *Advanced Organic Chemistry*: F. A. Carey and R. J. Sundberg. Plenum.
2. *A Guide Book to Mechanism in Organic Chemistry*: Peter Sykes, Longman/Pearson
3. Education.
4. *Mechanism and theory in Organic Chemistry*, T. H. Lowry and K. C. Richardson, Harper and Row.
5. *Reaction Mechanism in Organic Chemistry*: S. Mukherji and S. P. Singh, Macmillan publisher India.
6. *Advanced Organic Chemistry Reactions, Mechanism and Structure*: Jerry March. John Wiley and Sons.
7. *Structure and Mechanism in Organic Chemistry*: C. K. Ingold. Cornell University Press.
8. *A logical Approach to Modern Organic Chemistry*: Dr. Jagdamba Singh and Dr. S.
9. Anandvardhan. Pragati Prakasan.
10. *Stereochemistry, Conformation and Mechanism*: P. S. Kalsi, New Age International.

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

CO	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	PSO3	PSO 4
CHE102.1	Understand the mechanism, types of reactions and the factors affecting reactions	2					1	2		1		2
CHE102.2	Learn about the aliphatic nucleophilic Substitution reaction and corresponding name reactions	2		3			1	2	2	1		2
CHE102.3	Learn about the aromatic nucleophilic Substitution reaction and corresponding name reactions	2	2	2	3	1			2			1
CHE102.4	Apply concepts associated with these general reaction types to product prediction.	1	1						2			3
CHE102.5	Apply the concept of free radical reaction in predicting the product of the reaction	1		3	1			1	1			3

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

PAPER CHE 103: PHYSICAL CHEMISTRY I

Full Mark 100 (80 + 20)

Course Objectives:

To learn the mathematical concepts for solving eigenvalue and eigenvector problems in matrices and first and second order differential equations that are used for solving the time independent Schrodinger equation. Solve elementary model problems in quantum mechanics, particle in a potential-free box, particle on a ring, harmonic oscillator and demonstrate the solutions for hydrogen atom and molecular rotations and vibrations.

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

[CHE404.1]. pinpoint the historical aspects of development of quantum mechanics
[CHE404.2]. understand and explain the differences between classical and quantum mechanics
[CHE404.3]. understand the idea of wave function and the uncertainty relations
[CHE404.4]. solve Schroedinger equation for simple potentials
[CHE404.5]. spot, identify and relate the eigenvalue problems for energy, momentum, angular momentum and central potentials explain the idea of spin

B. SYLLABUS

UNIT 1 **Quantum I:** The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

UNIT 2 **Quantum II:** The Helium atom. The variation theorem, linear variation principle, Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Helium atom.

UNIT 3 **Quantum III:** Ordinary angular momentum, generalized angular momentum, eigen functions for angular momentum, eigenvalues of angular momentum, operator using ladder operators, addition of angular moments, spin, antisymmetry and Pauli exclusion principle**.** Multielectron atom. Electronic configuration. Russell-Saunders terms and coupling schemes, magnetic effects: spin- orbit coupling and Zeeman splitting.

UNIT 4 **Quantum IV:** H_2^+ and H_2 molecules: Valance bond theory (VBT) and molecular orbital theory (MOT) approaches. Homonuclear and Heteronuclear diatoms. Huckel theory of conjugated systems, bond order and charge density calculation. Applications to ethylene, butadiene, cyclopropenyl radical, and cyclobutadiene.

C. TEXT BOOKS

1. Molecular Thermodynamics, D. A. McQuarrie and J. D. Simon University Science Books, California
2. Quantum Chemistry: Ira N. Levine, Prentice Hall.

D. BOOKS FOR REFERENCES

1. Atkin's Physical Chemistry: P. W. Atkins, J. D. Paula, Oxford University Press
2. Statistical Mechanics, D. A. McQuarrie, University Science Books, California.
3. Statistical Mechanics - A Concise Introduction for Chemists B. Widom, , Cambridge University Press .
4. Statistical Thermodynamics: M. C. Gupta, New Age Pvt Publication

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

CO	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	PSO3	PSO 4
CHE404.1	pinpoint the historical aspects of development of quantum mechanics	3	1	1				1	1			2
CHE404.2	understand and explain the differences between classical and quantum mechanics	2	2	1					2			1
CHE404.3	understand the idea of wave function and the uncertainty relations	2	2			2		1	3	1		2
CHE404.4	solve Schröedinger equation for simple potentials	3	2		1	2		2	2			3
CHE404.5	spot, identify and relate the eigenvalue problems for energy, momentum, angular momentum and central potentials explain the idea of spin	3						2	2	2		3

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

PAPER CHE 104: ORGANIC SPECTROSCOPY
Full Mark 100 (80 + 20)

Course Objectives: To learn basic principles of NMR, IR, UV-Vis spectroscopy and mass spectrometry and to use these spectroscopic methods for organic structure elucidation.

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

[CHE304.1]. Apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.
[CHE304.2]. Interpret the above spectroscopic data of unknown compounds.
[CHE304.3]. Use these spectroscopic techniques in their research.
[CHE304.4]. Enhance employability as a spectro-chemist.

B. SYLLABUS

UNIT-1: (a)**Ultraviolet and Visible Spectroscopy:**

Various electronic transitions, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, dienes, conjugated polynes Fleser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.
(b)Infrared Spectroscopy
Instrumentation and sample handling, Characteristic vibrational frequencies of different organic compounds. Detail study of vibrational frequencies of compounds containing >C=O group. Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance, FTIR.

UNIT-2: Nuclear Magnetic Resonance Spectroscopy(^{1}H):

General principle of NMR, Chemical shift, spin-spin interaction, correlation for protons bonded to carbon and other nuclei, chemical exchange, effect of deuteration, first order and second order spectra, karplus curve. Simplification of complex spectra nuclear magnetic double resonance, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). Resonance of other nuclei.
Carbon-13 NMR Spectroscopy: General considerations, chemical shift (Aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbon), coupling constants. Two dimension NMR spectroscopy.

UNIT-3: Mass spectroscopy

Introduction, ion production – El, Cl, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometry. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination.

UNIT-4: **Spectroscopic Identification of Organic Molecules**:

Identification of organic compounds using modern techniques like UV, IR, ^{1}H NMR, ^{13}C NMR & Mass spectrometry.

TEXT BOOKS:

1. Silverstein, R. M.; Webster, F. X. *Spectrometric identification of organic compounds*; 6th /ed.; Wiley: New York, 1998.
2. Kemp, W. *Organic spectroscopy*; 3rd ed.; Macmillan Education: Houndmills, Basingstoke,Hampshire, 1991.

Reference Books:

1. Lambert, J. B; Shurvell, H. F, *Organic structural spectroscopy*, Prentice Hall, 1998.

2. Levitt, Malcolm H.; *Spin Dynamics-Basics of Nuclear Magnetic Resonance*, Second edition; John Willey & Sons Ltd.

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

CO	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAM SPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO3	PSO 4
CHE304.1	Apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.	2	1				2					3
CHE304.2	Interpret the above spectroscopic data of unknown compounds.	3	2	2	1			2	2	2	2	2
CHE304.3	Use these spectroscopic techniques in their research.	2		1	3		3	3			3	3
CHE304.4	Enhance employability as a spectro-chemist.	3			1							2

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

PAPER CHE 105: INORGANIC PRACTICAL

Full Mark 100

Course Objectives: The learners should be able to apply the principles of qualitative and quantitative analytical techniques in inorganic chemistry for compound identification and characterization.

1. QUALITATIVE ANALYSIS (Marks – 35)

Qualitative analysis of mixtures containing not more than six radicals / six radicals with any one of the following rare metals like tungsten, molybdenum, titanium and vanadium. (Organic radicals are excluded)

2. QUANTITATIVE ANALYSIS (Marks – 35)

Estimation major constituents of:-
(i) Chrome iron ore, (ii) white metal, (iii) pyrolusite, (iv) bronze (v) Complete 100 percent analysis of (a) dolomite or Portland cement and (b) brass

3. VIVA VOCE – 20 marks

4. RECORD – 10 marks

BOOKS FOR REFERENCES

1. Inorganic Experiments: J. Derck Woollins, VCH.
2. Microscale Inorganic-chemistry; Z.Szafran, RM. Pike and M.M.Singh. Wiley.
3. Practical Inorganic Chemistry: G.Marr and B.W. Rockett, van,Nostrand.
4. Vogel'-s Qualitative Inorganic Analysis (revised): G. Svehla, Longman.

SECOND SEMESTER

PAPER CHE 201: INORGANIC CHEMISTRY II

Full Mark 100 (80 + 20)

Course Objectives:

Apply the concept of linear combination of atomic orbitals to hybridization and directed bonding in polyatomic molecules. Show that molecular symmetry operations form a group and can be characterized by fundamental representations of groups known as irreducible representations. Apply the great orthogonality theorem to derive simple point groups and illustrate its use in the applications in crystal field theory and molecular spectroscopy. To identify and apply the concepts involved in the structure and physical properties of crystalline inorganic solids

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

[CHE 201.1]. Apply the concepts of symmetry and group theory in solving chemical structural problems.
[CHE 201.2]. Apply knowledge of group theory in spectroscopy.
[CHE 201.3]. Explain the different theories of bonding involving metal complexes.
[CHE 201.4]. Analyze modes of bonding in metal-metal multiple bonds and polysions.
[CHE 201.5]. Design and use new metal complex in environment friendly method.

B. SYLLABUS

UNIT 1 **Stereochemistry and bonding in main group compounds**: VSEPR, Walsh diagram (tri molecules), dz-Pp bonds, Bent rule and energetics of hybridization, some simple reactions of covalently bonded molecules.

UNIT 2 Symmetry and group theory: Symmetry operation, symmetry element, classification of symmetry elements, definition of group, subgroup, cyclic groups, molecular point groups, platonic solids, group multiplication table, matrix representation of symmetry elements, character of a representation, reducible and irreducible representation, the great orthogonality theorem (without proof).

UNIT 3 **Symmetry and spectroscopy:** Character table (explanation and significance), construction of character tables for C2v, C3v and C4v point groups, direct product, the standard reduction formula, Applications of group theoretical methods for selection rules in Infrared, Raman and electronic spectroscopy.

UNIT 4 **Solid state chemistry:** General idea of crystal lattice, unit cell, classification of crystals, crystal planes, Miller indices, Bragg's law and applications, determination of cubic crystal structure from systematic absences in diffraction pattern, perfect and imperfect crystals, point defects, Schottky defects and Frenkel defects, thermodynamics of Schottky and Frenkel defects, bonding in ionic solids, colour centers, non-stoichiometry defects, general idea of band theory of solids.

C. TEXT BOOKS

1. Chemical Application of Group Theory: F. A. Cotton, John Wiley.

D. BOOKS FOR REFERENCES

1. Symmetry in Chemistry: Orchin and Jaffe.
2. Group theory: K. V. Reddy, Tata McGraw Hill.
3. Introduction to Solid State Physics, C. Kettel, 7th edition, Wiley

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

CO	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	PSO3	PSO 4
CHE103.1	Apply the concepts of symmetry and group theory in solving chemical structural problems.	3	2	1	1		2	3	3	2	1	2
CHE103.2	Apply knowledge of group theory in spectroscopy.	2	1	2	1		3	2	3	2	2	3
CHE103.3	Explain the different theories of bonding involving metal complexes.	3	2	1	2		2	3	3	1	1	3
CHE103.4	Analyze modes of bonding in metal-metal multiple bonds and polysions.	3	2	1	1		3	3	3	1	1	2
CHE103.5	Design and use new metal complex in environment friendly method.	3	2	1	1		2	2	3	2	2	2

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

PAPER CHE 202: ORGANIC CHEMISTRY II

Full Mark 100 (80 + 20)

Course objective: To learn interpret the concept of aromaticity and the main properties of aromatic compounds and to learn the structure, stereochemistry of some name reactions, rearrangement reactions.

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

[CHE 202.1]. Understand the Conjugation, Cross conjugation, Hyperconjugation and Discuss the aromaticity
[CHE 202.2]. Learn about the stereochemistry, stereoselectivity and stereospecificity
[CHE 202.3]. Addition to carbon–carbon multiple bonds.
[CHE 202.4]. Learn about Elimination reactions and Discuss the nucleophilic substitution reactions.
[CHE 202.5]. Apply the concept of mechanism of molecular rearrangement reaction in predicting the product of the reaction

B. SYLLABUS

UNIT 1 **Nature of Bonding in Organic Molecules:** Delocalized chemical bonding: conjugation, cross conjugation, resonance, hyperconjugation, tautomerism. Aromaticity in benzenoid and nonbenzenoid compounds, alternant and non-alternant hydrocarbons. Huckel's rule, energy level of π-molecular orbitals, annulenes, antiaromaticity, homoaromaticity,

UNIT 2 Stereochemistry Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity. Chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical purity, stereospecifjc and, stereoselective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon.

UNIT 3 (a) Addition to Carbon-Carbon Multiple Bonds:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, selectivity, orientation and reactivity, Electrophilic cyclization, Baldwin's rule. Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration, Michael reaction.

(b) Addition to Carbon-Hetero Multiple Bond

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds. Wittig reaction. Mechanism of condensation reactions involving enolates, Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions.

UNIT 4 (a) Elimination Reactions:

The E2, EI and E1cB mechanisms. Orientation of the double bond. Reactivity: Effects of substrate structures, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination.

(b)Molecular Rearrangements

General mechanistic considerations: nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii , Arndt-Eistert synthesis, Neber, Beckmann, Hofmann, Curtius, Schmidt,

C. TEXT BOOKS

1. Organic chemistry: J. Clayden, N. Greeves, S. Warren and P. Wothers, Oxford University Press.

D. BOOKS FOR REFERENCES

1. *Advanced Organic Chemistry Reactions, Mechanism and Structure*: Jerry March. JohnWiley and Sons.
2. *Advanced Organic Chemistry*: F. A. Carey and R. J. Sundberg. Plenum.
3. *A Guide Book to Mechanism in Organic Chemistry*: Peter Sykes, Longman/Pearson
4. Education.
5. *Structure and Mechanism in Organic Chemistry*: C. K. Ingold. Cornell University Press.
6. *A logical Approach to Modern Organic Chemistry*: Dr. Jagdamba Singh and Dr. S.
7. Anandvardhan. Pragati Prakasan.
8. *Reaction Mechanism in Organic Chemistry*: S. Mukherji and S. P. Singh, Macmillan publisher India.
9. *Stereochemistry of Organic Compounds*: D. Nasipuri, New Age International.
10. *Stereochemistry of Organic Compounds*: P. S. Kalsi, New Age International.
11. *Stereochemistry of Organic Compounds*: E. L. Eliel and S. H. Wilen. John Wiley.
12. *Stereochemistry, Conformation and Mechanism*: P. S. Kalsi, New Age International.

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

CO	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	PSO3	PSO 4
CHE202.1	Understand the Conjugation, Cross conjugation, Hyperconjugation and Discuss the aromaticity	1					1	2		1		2
CHE202.2	Learn about the stereochemistry, stereoselectivity and stereospecificity	1		1			1	2	2	1		2
CHE202.3	Addition to carbon–carbon multiple bonds.	2		2				1	2			1
CHE202.4	Learn about Elimination reactions and Discuss the nucleophilic substitution reactions.	2						1	2			1
CHE202.5	Apply the concept of mechanism of molecular rearrangement reaction in predicting the product of the reaction	2		1	1			1	1			1

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

PAPER CHE 203: PHYSICAL CHEMISTRY II
Full Mark 100 (80 + 20)

Course Objectives: The learners should be able to apply theories in electrochemistry to analyze electrode kinetics. The learners should be able to apply elementary laws of chemical kinetics and analyze reaction mechanisms and changes in transport properties of chemical reactions and collision processes

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

[CHE303.1]. Discuss the electrical double layer and metal/electrolyte interface.
[CHE303.2]. Learn about kinetic equivalence terms and theories of reaction rates.
[CHE303.3]. Discuss the Elementary gas phase reactions and Fast reaction kinetics.
[CHE303.4]. Understand the Chain reactions, Acid Base Catalysis.

B. SYLLABUS

Unit-1. Electrochemistry I: Interionic attraction theory and Debye-Huckel treatment, derivation of Onsager limiting law and its verification and modification, determination of dissociation of electrolytes. Activities, activity coefficients, Debye-Huckel treatment, Debye-Huckel-Bronsted equation, Salt effect, Determination of activity coefficients from solubility method, freezing point method, EMF method. Ion association, Determination of thermodynamic dissociation constant of weak electrolytes by Shedlovsky method and by EMF method, reversible cells, chemical and concentration cells, liquid junction potential, single electrode potential, oxidation and reduction electrodes.

Unit-2. Electrochemistry II: Factors affecting EMF of half cells, Electrolytic polarization, decomposition potential and Over voltage. Electrocatalysis-influence of various parameters. Diffusion layer. The limiting current density and its practical application. Corrosion: Introduction to corrosion, homogenous theory, forms of corrosion, corrosion monitoring and prevention methods.

Unit-3. Kinetics I: (a)Methods of determining rate laws, Temperature dependence of reaction rates, Collision theory of collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation Activated complex theory; kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions, Lindemann reaction.

Unit-4. Kinetics II: **Kinetics of complex reactions:** Opposing, Parallel, Consecutive reactions. Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane). Kinetics of Catalytic Reactions: Acid-base Catalysis, Enzyme Catalysis, Homogeneous & Heterogeneous Catalysis. Fast reactions: General feature, Study of Fast reactions by relaxation, Stopped flow and Flashphotolysis.

C. TEXT BOOKS

1. Modem Electrochemistry: Vol.-I and Vol. II, J. O. M. Bockris and A. K. N. Reddy, Plenum.
2. Elements of Physical Chemistry P W Atkins, Julio de Paula, Oxford University Press

D. BOOKS FOR REFERENCES

1. An Introduction to electrochemistry: S. Glasstone, Affiliated East-West Press Pvt. Ltd.
2. Physical Chemistry by D.N. Bajpai
3. Principles of Physical Chemistry by B. R. Puri, L. R. Sharma & M. S. Pathania, Shoban Lal Nagin Chand& Co.

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

CO	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	PSO3	PSO 4
CHE303.1	Apply NMR, IR, MS, UV-Vis spectroscopic techniques in solving structure of organic molecules and in determination of their stereochemistry.	2	1		1		2					3
CHE303.2	Interpret the above spectroscopic data of unknown compounds.	3		2	3		2	2	2	2	1	2
CHE303.3	Use these spectroscopic techniques in their research.	3		3	1		3	3			1	3
CHE303.4	Enhance employability as a spectro-chemist.	3			1		2					2

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

PAPER CHE 204: BIOINORGANIC AND SUPRAMOLECULAR CHEMISTRY

Full Mark 100 (80 + 20)

Course objectives: The learners should be able to apply, analyze and evaluate the active site structure and functions of some transition metal ion containing metalloproteins or enzymes. The course will provide a fundamental aspect in supramolecular systems and give students an awareness and appreciation of the wider aspects of chemistry and functional materials accessible through combination and assembly of organic, inorganic, coordination and biological molecules.

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

[CHE204.1]. Biomolecules: types, structure, functions in cellular life and importance in context with day to day life.
[CHE204.2]. Learn about fundamentals of supramolecular chemistry.
[CHE204.3]. Understand the concept of coenzymes & cofactors, kinetics, mode of action, classification and role in different biological processes.
[CHE204.4]. Enhance employability as a material chemist.

B. SYLLABUS

UNIT 1 **Biomolecules and their Roles in Metal Ions Storage and Transportation:** A brief introduction to bio-inorganic chemistry. Biologically important metal ions (Na, K, Mg, Ca, Cu, Fe, Zn, Co and Mo) and their functions. Mechanism of transport of metal ions through biological fluids and membranes, different types of passive and active transport processes and their mechanism, Na+/K+ pump, calcium pump, and ionophores. Metal ion transport and storage: Ferritin, Transferrin and siderophores.

UNIT 2 Role of Proteins as Oxygen and Electron Carriers: Oxygen transport and storage: Hemoglobin, myoglobin, and their behavior as oxygen carrier, O_2 affinity, cooperativity and Bohr's effect, hemerythrin, hemocyanin. Oxygen activation: Cytochrome P450, Cytochrome c oxidase. Electron Transfer: Cytochromes, Iron-Sulfur Proteins (rubredoxins and ferrodoxins) and Copper Proteins
Magnesium porphyrins (Chlorophyll): Photosynthesis, the light and dark reaction (Calvin cycle).

UNIT 3 Biomolecular Catalysis: Preliminary idea about enzyme catalysis. Enzyme-substrate binding problem, carboxypeptidase, carbonic anhydrase. Other metal containing enzymes: Catalase, peroxidase, superoxide dismutase, alcohol dehydrogenase, xanthine oxidase, vitamin B12 coenzyme, photosystem I and II, oxygen evolving center

Nitrogen fixation: Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence.

UNIT 4 **Supramolecular Chemistry:** Fundamentals of Supramolecular Chemistry. Intermolecular forces: ion pairing, ion dipole and dipole dipole interactions, hydrogen bonding, cation-pi, anion –pi, pi-pi interactions and Van der Waal forces. Solvation and hydrophobic effect. Molecular recognition Principle, host guest complementarity, preorganization, chelate effect, cooperativity, synthesis and applications of supramolecular host (crown ethers, lariat ethers, podands, cryptands, spherands, calix[n]arenes, cyclodextrin) as cation and anion binding receptors and for ion pair recognition.

Biological supermolecules: ion channels, information conversion and amplification, energy conversion, material conversion, cleaving genes.

C. TEXT BOOKS

1. S. J. Lippard and J. M. Berg, Principle of Bioinorganic Chemistry, University Science Books (1994)
2. Supramolecular Chemistry, J. W. Steed and J. L. Atwood, Willey, 2nd Ed.

D. BOOKS FOR REFERENCES

1. Bioinorganic Chemistry I. Bertini, H. B. Gray, S. J. Lippard, J. S. Valenting, University Science Books.

2. Bioinorganic Chemistry, Asim Kumar Das, Books & Allied (P) Ltd. 1st ed. 2015.
3. Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi, J.P. Kalsi, New Age International

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

CO	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	PSO3	PSO 4
CHE203.1	Biomolecules: types, structure, functions in cellular life and importance in context with day to day life.	1					1	1				2
CHE203.2	Learn about fundamentals of supramolecular chemistry.	3	1	1								1
CHE203.3	Understand the concept of coenzymes & cofactors, kinetics, mode of action, classification and role in different biological processes.	1	2	2		2		1		1		2
CHE203.4	Enhance employability as a material chemist.	2	2	1	1	2			2			3
CHE203.5	Biomolecules: types, structure, functions in cellular life and importance in context with day to day life.	2							2	2		3

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

PAPER CHE 205: ORGANIC PRACTICAL
Full Mark 100

Course Objectives: The learners should be able to: Apply principles of separation and isolation techniques in organic reactions. Analyze and synthesis of organic compounds

1. Separation, purification and identification of organic compounds having at least two functional groups.

2. Quantitative Analysis:

(a) Estimation of Anilines / Phenols using hromate bromide solution.
(b) Determination of Iodine and Saponification values of an oil sample.
(c) Estimation of Keto group.
(d) Determination of iodine value and saponification value of an oil sample.

3. Organic Synthesis:

(a) Preparation of Anthranilic acid
(b) Preparation of Methyl Orange
(c) Preparation of Adipic acid by chromic acid oxidation of cyclohexanol.
(d) *p*-chloro toluene from p-toluidine (Sandmeyer reaction)
(e) Synthesis of p-nitroaniline & p-bromo aniline (Aromatic electrophilic substitution)
(f) Synthesis of triphenyl methanol from benzoic acid (Grignard reaction)

BOOKS FOR REFERENCES

1. The Systematic Identification of Organic Compounds: R.L. Shriner, C. K. F. Harmann, T.C. Morrill,
2. D.Y. Curtin, R.C. Fusion, John Wiley and Sons.
3. Organic Analytical Chemistry (Theory and Practice): Jagmohan, Narosa Publishing House.
4. A Text Book of Practical Organic Chemistry: Arthur I.Vogel, .E.L.B.S. and Longman.
5. Experiments and Techniques in Organic Chemistry: D. Pasto, C. Johnson.
6. Systematic Qualitative Organic Analysis: H. Middleton, Orient Longman.
7. Hand Book of Organic Analysis, Qualitative & Quantitative, M.T.Clarke, Edward Arnold (Publisher).
8. Vogel's Text Book of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
9. A Text Book of Practical Organic Chemistry (Qualitative). Arthur I.Vogel Haynes, Arnold Publishers.

PAPER CHE 206 A: ANALYTICAL CHEMISTRY
Full Mark 100 (80 + 20)

UNIT 1 **Error analysis**

Data Analysis: Uncertainties, errors, mean, standard deviation, least square fit, testing the fit (C2 test, residual etc.). Signal to noise ratio.

UNIT 2 **Spectral methods**

(a) ORD: Terminology, cotton effect, ORD of ketones, axial halo ketone rule
(b) Mossbauer spectroscopy: Principles of Mossbauer spectroscopy, Experimental methods, Theoretical aspects, Quadrupole splitting, magnetic hyperfine interaction
(c) Mass spectroscopy (only principles)
(d) PES, XPS, Auger electron Spectroscopy, AAS (only principles)

UNIT 3 **Thermoanalytical**

Thermogravimetric analysis (TGA): Principle, instrumentation, factors affecting TGA curve, derivative thermogravimetric analysis (DTGA) and application of thermogravimetric analysis, Differential thermal analysis (DTA), instrumentation of DTA and application of DTA, Simultaneous study of TGA, DTA with examples. Differential scanning calorimetry (DSC) and thermometric titration

UNIT 4 **Electroanalytical**

Classification of electroanalytical methods, principles and applications of voltammetry, cyclic voltammetry, anodic stripping voltammetry, polarography, amperometry, coulometry, conductometry and ion selective electrodes.

TEXT BOOKS

BOOKS FOR REFERENCES

1. Basic Principle of Analytical Chemistry by S.M. Khopkar
2. Analytical Chemistry, 7th Edition by Gary D. Christian, P K. Dasgupta, K. A. Schug, Wiley

PAPER CHE 206 B: SURFACE CHEMISTRY AND CATALYSIS
Full Mark 100 (80 + 20)

UNIT 1: Structural aspects of organized molecular assemblies, surfactants, classification of surfactants, micelles, critical micellar concentration, different methods for determination of critical micellar concentration, thermodynamics of micellization, aggregation number, reverse micelles, microemulsion (oil in water and water in oil).

UNIT 2: Surface Tension, Capillary Action, Adsorption, Types of Adsorption, Physisorption, Chemisorption, Gibbs Adsorption Isotherm, Freundlich's Adsorption Isotherm, Langmuir's Adsorption Isotherm, BET Adsorption Isotherm and its Applications, Heat of Adsorption, Estimation of Surface Areas of Solids from Solution Adsorption Studies.

UNIT 3: Homogeneous and Heterogeneous Catalysis.Acid-base Catalysis, Enzyme Catalysis, Enzyme kinetics, michaelismenten and lineweaver-burk plots, phase transfer catalysis. Evaluation ofactivity and selectivity of catalysts.

UNIT 4: Catalysts acido-baseic, hydrogenation dehydrogenation, oxidation-reduction, Zeolite. Mechanisms of catalyzed reactions. Examples of catalysts applications – cracking, alkylation, hydrogenation, hydration and dehydration processes. Modern sorption and spectral methods of characterization of catalysts.

TEXT BOOKS

1. Introduction to Surface Chemistry and Catalysis by Gabar A. Somorjai (John Wiley & Sons)

BOOKS FOR REFERENCES

2. Physical Chemistry of Macromolecules by C. Tanford CH

PAPER CHE 206 C: COMPUTATIONAL CHEMISTRY AND MOLECULAR MODELLING
Full Mark 100 (80 + 20)

UNIT 1: Molecular mechanics – Vibrational motion, normal modes of vibration, the quantum mechanical treatment, the taylor expansion, the morse potential, more advanced empirical potential, molecular mechanics, professional molecular mechanics force fields, a sample MM calculation, General features of potential energy surfaces.

UNIT 2: The LCAO procedure, the electronic energy, the koopmans theorem, open-shell system, unrestricted Hartree-Fock theory, the J and K operator, Bond lengths and the Huckel model, molecular mechanics and pi-electron systems, alternant hydrocarbons, treatment of heteroatoms, Extended Huckel theory.

UNIT 3: Basic sets – Introduction, the energy calculation from the STO function, the energy calculation of multielectron systems, Gaussian type orbitals, Difference between STOs & GTOs, classifications of basis sets, A comparison of energy calculation of the Hydrogen atoms based on STO-2G, STO-3G & STO-^G basis sets, contracted Gaussian type orbitals, Double and Zeta basis sets and split Valence basis sets, polarized basis sets.

UNIT 4: Semiempirical methods – Introduction, NDO, CNDO, MNDO, AM1 & PM3 methods, Ab Intio Method – Introduction, level of theory, geometry input, An Ab-intio HF-LCAO calculation, computation of the correlation energy, Density Functional Theory – Introduction, electron density, pair density,

development of DFT, the kohn and Sham method, density functionals, the Lee, Yang and Parr correlation energy functional and the potentials, DFT methods, application of DFT method.

TEXT BOOKS

1. Modelling Molecular structures _ Alan Hinchliffe, John Wiley & sons, ltd

BOOKS FOR REFERENCES

2. Electron Density theory of atoms and molecules-N. H. March, Academic press, London

THIRD SEMESTER

PAPER CHE 301: INORGANIC CHEMISTRY III

Full Mark 100 (80 + 20)

Course Objectives: The learners should be able to apply theories of chemical bonding, reaction mechanism, electronic structure and magnetic properties of coordination complexes to identify the occurrence.

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

[CHE301.1]. Identify the principles, structure and reactivity of selected coordination complexes
[CHE301.2]. Interpret their electronic spectra and magnetic properties.
[CHE301.3]. Utilize the principles of transition metal coordination complexes in understanding functions of biological systems.
[CHE301.4]. Apply different electron counting rules to predict the shape/geometry of low and high nuclearity metal carbonyl clusters

B. SYLLABUS

UNIT 1 **Electronic spectra of transition metal complexes:** Spectroscopic ground states, Orgel diagrams for d1-d9 states in Oh and Td symmetry, Tanabe- Sugano diagrams for d^2 configuration in Oh and Td symmetry. Calculations of Dq, B and β parameters.

UNIT 2 **Metal ligand bonding:** Crystal Field Theory and its limitations, Elementary idea of Angular overlap model, Molecular orbital theory for octahedral, tetrahedral and square planar complexes, σ and π -bonding in molecular orbital theory.

UNIT 3: **Metal π –Complex:** Preparation, Bonding, Structure and Important Reactions of Transition metal carbonyls, nitrosyls, cabonyl hydrides, isolobal analogy, dioxygen and dinitrogen compounds. **Metal clusters:** Metalloboranes, Metallocarboranes, Metal carbonyls and Metal halide clusters.

UNIT 4 **Metal ligand equilibrium in solutions:** Stepwise and Overall formation constants and their interaction, trends in stepwise constants. Factors affecting the Stability of metal complexes with reference to the nature of metal ion and ligand. Chelate effect, Macrocyclic effect and its thermodynamic origin. Determination of BinaryFormation Constants by pHmetry and Spectrophotometry.

C. TEXT BOOKS

1. Inorganic Chemistry: Principles of Structure and Reactivity by J. E. Huheey, E. A. Keiter and R. L. Keiter, 4th ed. Harper Collins 1993
2. Inorganic Chemistry by D. F. Shriver and P. W. Atkins, 3rd Ed., Oxford.

D. BOOKS FOR REFERENCES

1. Advanced Inorganic Chemistry by F. A. Cotton, G. W. Wilkinson, 5th edition, John-Wiley & Sons, 1988.
2. Comprehensive Coordination Chemistry eds.: G. Wilkinson, R. D. Gillars and J.A. McCleverty, Pergamon.
3. Inorganic chemistry: Gary L. Miessler, Donald A. Tarr, Pearson

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

CO	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	PSO3	PSO 4
CHE301.1	Identify the principles, structure and reactivity of selected coordination complexes	3	1		1		2					3
CHE301.2	Interpret their electronic spectra and magnetic properties.	3			2		2		1	2	1	2
CHE301.3	Utilize the principles of transition metal coordination complexes in understanding functions of biological systems.	2	1		2		3				1	2
CHE301.4	Apply different electron counting rules to predict the shape/geometry of low and high nuclearity metal carbonyl clusters	2			2		2		2	2		2

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

PAPER CHE 302: ORGANIC CHEMISTRY III

Full Mark 100 (80 + 20)

Course Objectives: To learn and understand the orbital interactions (Woodward Hoffmann rules) in concerted reactions. Learn to apply concerted and stepwise reactions in organic synthesis To learn various organic reactions and reagents used in them as tools applied in the art of organic synthesis. To learn retrosynthetic approach towards organic synthesis

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

[CHE302.1]. Comprehend the structure-reactivity pattern of reactive intermediates involved in organic reactions.
[CHE302.2]. Comprehend the orbital interactions and orbital symmetry correlations of various pericyclic reactions.
[CHE302.3]. Write the mechanism of organic reactions involving reactive intermediates and concerted processes.
[CHE302.4]. Apply these reactions in organic synthesis.

B. SYLLABUS

UNIT-1: Pericyclic reaction-I
Molecular orbitals of ethylene, 1,3–butadiene, 1,3,5–hexatriene and, conjugated system with odd number of carbon atom. Assignment of symmetry of molecular orbitals with respect to mirror plane and C2 axis. Classification of pericyclic reactions. Woodward – Hoffmann correlation diagrams. FMO and Transition state aromaticity method, Electrocyclic reactions – conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems. Cycloadditions – antarafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolar cycloadditions and cheletropic reactions.
UNIT- 2: Pericyclic reaction – II
Sigmatropic rearrangements – suprafacial and antarafacial shifts of H, sigmatroic shifts involving carbon moieties, 3,3– and 5,5–sigmatropic rearrangements. Claisen, Cope and Aza-Cope rearrangements. Fluxional tautomerism. Ene reaction.
UNIT-3: Disconnection approach – I
An introduction to synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, the importance of the order of events in organic synthesis, one group C-X and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis.
Oxidation
Introduction, Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated) and other organic compounds with functional group. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium(III)nitrate.
Reduction
Introduction. Different reductive processes. Hydrocarbons. Carbonyl compounds, acids and their derivatives. Epoxides. Nitro, nitroso, azo and oxime groups. Hydrogenolysis.

UNIT-4: Disconnection approach – II
Protecting Groups, Principle of protection of alcohol, amine, carbonyl and carboxyl groups.
One Group C-C Disconnection
Alcohols and carbonyl compounds, regioselectivity, Alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis.
Two Group C-C Disconnections
Diels-Alder reaction, 1,3-difunctionalised compounds, α,β- unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalised compounds. Michael addition and Robinson annulation.

C. TEXT BOOKS

1. Modern Methods of Organic Synthesis, 4th Edition, W. Carruthers and Iain Coldham, Cambridge University Press, 2004.
2. Organic Synthesis: The Disconnection Approach, Stuart Warren, John Wiley & Sons, 2004
3. Photo Chemistry and Pericyclic Reactians: Jagdamba Singh and Jaya Singh, New Age International.

D. Reference Books:

1. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Part A and B Springer, 5th Ed.(2005)
2. Pricyclic Reactions S.M. Mukherjee, Mc millan India
3. Modern Synthetic Reactions: Second Edition, H. O. House, Benjamin, Menlo Park, 1972.
4. Principles of Organic Synthesis, R.O.C. Norman & J. M. Coxon, 3rd Edn., Nelson Thornes

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

CO	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	PSO3	PSO 4
CHE302.1	Comprehend the structure-reactivity pattern of reactive intermediates involved in organic reactions.	2	1		1		2					3
CHE302.2	Comprehend the orbital interactions and orbital symmetry correlations of various pericyclic reactions.	3					2	2	1	2	1	2
CHE302.3	Write the mechanism of organic reactions involving reactive intermediates and concerted processes.	3	1		1						1	2
CHE302.4	Apply these reactions in organic synthesis.	2			1		2					2

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

PAPER CHE 303: MOLECULAR SPECTROSCOPY

Full Mark 100 (80 + 20)

Course Objectives:

Recognize the fundamental principles of optical and magnetic resonance through both theory and examples drawn from molecular literature, and show that spectroscopy connects matter with molecules through interaction of electromagnetic radiation.

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

[CHE203.1]. Understand the concepts of spectroscopy
[CHE203.2]. Understand Microwave Spectroscopy and their applications for chemical analysis.
[CHE203.3]. Understand Infrared-Vibration-rotation Spectroscopy and their applications for chemical analysis.
[CHE203.4]. Apply Raman Spectroscopy for chemical analysis
[CHE203.5]. Apply the concept of Electronic spectroscopy of different elements and simple molecules, and for organic compounds analysis, medical diagnostics.

B. SYLLABUS

UNIT 1**Introduction to EM radiation:** Interaction of light wave with matter, electromagnetic spectrum, basic concept of spectroscopy **Microwave Spectroscopy** Theory of microwave spectroscopy, Interaction of microwave region radiation with matter, rotational spectra of diatomic molecule (rigid rotor model), selection rule, Classification of molecules depending on relation among moment of Inertia, determination of bond length of a diatomic molecule using the application of microwave spectroscopy

UNIT 2 **Vibrational spectroscopy:** Theory of IR spectroscopy, types of vibrations, vibrational frequency, The vibration of diatomic molecule (harmonic oscillator), force constant and bond strength, Anharmonicity, Morse potential energy diagram, selection rule, Normal modes of vibrations, finger print region

UNIT 3 **Raman spectroscopy:** Theory of Raman spectra, Rotational Raman spectra, Vibrational Raman spectra, Rotational- Vibrational Raman spectra, Stokes' line, Anti-stokes' line, R branch, S branch, selection rules, Rule of mutual exclusion.

UNIT 4 **Electronic spectroscopy:** Electronic transitions, Type of electronic transitions, Born-Oppenheimer approximation, Franck- Condon principle, Vertical transitions, Selection rules, Beer-Lambert law, Limitation of Beer lambert law, Absorption, Fluorescence, Phosphorescence, delayed fluorescence, Jablonski diagram**.**

C. TEXT BOOKS

1. Fundamentals of Molecular Spectroscopy: C. N. Banwell, McGraw-Hill.
2. Fundamentals of Molecular Spectroscopy, G.M. Barrow

D. BOOKS FOR REFERENCES

1. Basic Principles of Spectroscopy: R. Chang, Mc Graw Hill
2. Elementary Organic Spectroscopy, Y.R. Sharma 5th Edition, S. Chand & Sons.
3. Molecular Spectroscopy, P.S. Sindhu
4. Physical Chemistry through problems, Dogra and Dogra

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

CO	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	PSO3	PSO 4
CHE203.1	Understand the concepts of spectroscopy	1					1	2				2
CHE203.2	Understand Microwave Spectroscopy and their applications for chemical analysis.	3	1	1			1	2	2			2
CHE203.3	Understand Infrared-Vibration-rotation Spectroscopy and their applications for chemical analysis.	3	2	2		2		1	2	1		1
CHE203.4	Apply Raman Spectroscopy for chemical analysis	2	2			2			2	1		1
CHE203.5	Apply the concept of Electronic spectroscopy of different elements and simple molecules, and for organic compounds analysis, medical diagnostics.	1		1	1				1	1		1

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

PAPER CHE 304: MATERIAL CHEMISTRY

Full Mark 100 (80 + 20)

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

[CHE104.1]. Interpret the future-oriented field of material chemistry for global importance.
[CHE104.2]. Understand the process of polymerization and Implement the concept of polymer science in various fields.
[CHE104.3]. Differentiate various nanomaterials, carbon-based materials and their industrial importance.
[CHE104.4]. Prepare advance materials by applying the concept of Organized Assemblies and micellar chemistry.

B. SYLLABUS

UNIT 1 **Polymer I:** Introduction to Polymer Science: Definition of Polymers, Degree of Polymerization, Nomenclature and classification of polymers, Natural & Synthetic polymers, Homopolymer and Copolymers, Polymerization process, Addition and Condensation polymerization. Addition Polymerization: Introduction, Monomers of Addition polymers, Free radical initiators, Polymerization mechanism, Steady-state kinetics of Radical Polymerization, Determination of molecular weight by viscosity method.
UNIT 2 **Polymer II:** Condensation Polymerization: Nylon 6, Nylon 6.6, Polyester, Phenol- formaldehyde resins, Epoxy resins, Polysiloxane, Amino resins, Melamine- formaldehyde Polymers. Co-polymerization: Classification of copolymer, The copolymer equation, Kinetics of Copolymerization, Mayo and Lewis equation, Determination of Monomer reactivity ratios, Fineman and Ross method, Graft Copolymer.
UNIT 3 **Nanomaterial and nanoscience:** Introduction and concepts of Nanomaterials and nanoscience, Different types of nanomaterials including nanocomposites and nanoporus materials- shapes, structure and properties. Quantum mechanics and Jellium model of nanosystems, electrical and magneticproperties of nanoparticles. Nanostructured. Carbon based materials: Fullerene, carbon nanotube, graphene, carbon nanobuds, synthesis and application of carbon nanotubes. Characterization Techniques of Nanomaterials: Scanning probe microscopy, scanning electron microscopy, Transmission electron microscopy, Xray diffraction.
UNIT 4 Organized assemblies: Surfactants, classification of surfactants, micelles, critical micellar concentration, different methods for determination of critical micellar concentration, thermodynamics of micellization, aggregation number, reverse micelles, microemulsion (oil in water and water in oil), Cyclodextrin, Lipids, Liposome

C. TEXT BOOKS

1. Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
2. Shriver D. E.,Atkins P. W., InorganicChemistry, Oxford UniversityPres ,5thEdn..

D. BOOKS FOR REFERENCES

1. Principle of Polymer Science - Paul J. Flory.
2. Nayak P.L., Polymer Chemistry, Kalyani Publisher (2017).
3. Nanomaterials and Nanochemistry- C Brechignac, P. Houdy, M Lahmani , Springer
4. An Introduction to Nanomaterials and Nanoscience- Asim K Das.

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

CO	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	PSO3	PSO 4
CHE104.1	Interpret the future-oriented field of material chemistry for global importance.	2					1	2	1	1	2	2
CHE104.2	Understand the process of polymerization and Implement the concept of polymer science in various fields.	2	2			1		2	1	3	3	3
CHE104.3	Differentiate various nanomaterials, carbon-based materials and their industrial importance.	1			2		1		1			2
CHE104.4	Prepare advance materials by applying the concept of Organized Assemblies and micellar chemistry.	1			2		2		2	2		2

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

PAPER CHE 305: PHYSICAL PRACTICAL
Full Mark 100

Course Objectives: The learners should be able to validate the conceptual understanding acquired from the theory classes.

Kinetics of ester hydrolysis by acids and alkali.
Adsorption: Adsorption of acetic acid on animal charcoal and verification of Freundlich isotherm.
Study of the surface tension – concentration relationship for solutions (Gibb's equation)
Phase equilibria: Determination of critical solution temperature of phenol-water system.
Construction of phase diagram for a three component system (chloroform-acetic acid –water).
Electrochemistry: Determination of strength of strong acid and weak acid in given mixture conductometrically.
Potentiometric titration of a strong acid with strong base using quinhydrone electrode.
pH metric and conductometric titrations: 1. Determination of strength of strong acid by titrating with strong base / weak base.
Photochemistry: 1. Verification of Beer Lambert law.
Polarimetry: 1. Study of the kinetics of Hydrolysis of cane sugar.

BOOKS FOR REFERENCES

1. Experimental physical chemistry: R. C. Das and B. Behera, Tata McGraw Hill.
2. Findlay's practical chemistry (revised): B. P. Levitt, Longman.
3. Advanced practical physical chemistry: J. B. Yadav, Goel publishing house, Meerut.

PAPER CHE 306 A: ENVIRONMENTAL CHEMISTRY
Full Mark 100 (80 + 20)

UNIT I

Environment Introduction, Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, Biogeochemical Cycles of C, N, P, S and O. Biodistribution of elements.

Hydrosphere Chemical composition of water bodies-takes, streams, rivers and wet lands etc. Hydrological cycle. Aquatic pollution-inorganic, organic, pesticide agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters- dissolved oxygen, biochemical oxygen demand, solids, metalsm, content of chloride, sulphate, phosphate, nitrate and mocro-organisms. Water quality standards, Analytical methods for measuring BOD, DO, COD, F, oils,metals (As, Cd, Cr, Hg, Pb, Se etc)residual chloride and chlorine demand. Purification and treatment of water.

UNIT II

Soils composition, micro and macro nutrients, pollution-fertilizers, pesticides, plastics and metals, waste treatment

Atmosphere Chemical composition of atmosphere-particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Greenhouse effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

UNIT III

Industrial Pollution Cement, Sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

UNIT IV

Environmental Toxicology, Chemical solutions to environmental problems, biodegradability, principles of decomposition.

TEXT BOOKS

1. Environmental Chemistry, A. K. De, Wiley Eastern

BOOKS FOR REFERENCES

1. Environmental Chemistry, S.E. Manahan, Lewis Publishers
2. Environmental Chemistry with Green Chemistry, A. K. Das, Books & Allied (P) Ltd., Kolkata, 1st Edn, 2010
3. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication

PAPER CHE 306 B: INDUSTRIAL PROCESS
Full Mark 100 (80 + 20)

UNIT-I:

Petroleum and coal based chemicals: Composition of petroleum, cracking processes, Commercial production of ethylene, acetylene, polymerization mechanisms, addition, condensation, step growth, chain growth, method of polymerization, distillation of coal.

UNIT – II

(a)oil based industries: oils and fats: solvent extraction of oils, hydrogenation of oil, use of oil in the manufacturing of soap, paints and varnishes. (b) Surface active agents: classification and manufacturing of detergents used for clinging purposes. (c) Fermentation industries: a general Discussion On fermentation conditions, manufacturing of pencillin.

UNIT – III:

Pesticides, battery and explosives:

Origin of pesticides and uses, origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite(RDX), Introduction to rocket propellant, primary and Secondary batteries, battery components and their role, characteristics of battery, fuel cells, solar cells.

UNIT –IV

Pharmaceutical industries – Manufacturing of compounds of pharmaceutical importance.

TEXT BOOKS

1. Outlines of chemical Technology by M. Gopala Rao and Marshall Sittig,

PAPER CHE 306 C: MATTER AND ENERGY BALANCE
Full Mark 100 (80 + 20)

UNIT I

Material Balance (a) Material Balances Without Chemical Reactions: Process Flow-Sheet, Material Balances, Recycling Operations, Material Balances of Unsteady State Operations

UNIT II

Material Balances Involving Chemical Reactions, Definition of Terms, Electrochemical reactions, recycling, parallel and Bypassing Operations, Metallurgical Applications.

UNIT III

Energy balance Energy and Thermo-Chemistry, Energy Balances, Heat capacity, Heat Capacity of Gases at Constant Pressure, Sensible Heat Changes in Liquids, Heat Capacity of Gaseous Mixtures, Latent Heats, Enthalpy Changes During Phase Transfer Accompanied by Sensible heat Changes, Enthalpy Changes Accompanying Chemical Reactions, Effect of temperature on Heat of Foremation, Heat of reaction, Adiabatic reactions, Effect of Pressure on Heat of reaction, Thermochemistry of Mixing Process, Dissolution of Solids, Liquid-liquid mixtures, heat of Solution by partial Molal Quantities.

UNIT IV

Stoichiometry and Unit Operations Distillation, Absoption and Stripping, Extraction and Leaching, Crystallisation, psychrometry, drying, Evaporation, Less Conventional Operation.

TEXT BOOKS

1. Stochiometry by I Bhatt and S. M. Vora (Tata McGaw Hill, new Delhi)

FOURTH SEMESTER

PAPER CHE 401: INORGANIC CHEMISTRY IV

Full Mark 100 (80 + 20)

Course Objectives: The learners should be able to analyze the mechanism of selected catalytic organic reactions from the structure-bonding aspects and reactivity of simple organometallic compounds

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

[CHE401.1]. Learn about the interdisciplinary character of organometallic chemistry among the conventional branches of chemistry as well as the industrial aspects of organometallic chemistry
[CHE401.2]. Understand the chemical processes involved in the various renowned industrial conversions (e.g Olefin polymerization, Hydrogenation, etc.) carried out in presence of organometallic complexes
[CHE401.3]. Apply knowledge of metal-ligand bond interaction in explaining reactions of metal complexes.
[CHE401.4]. Apply the concept of Electronic spectroscopy for inorganic compounds analysis.

B. SYLLABUS

UNIT 1 Reaction mechanisms: Energy profile of a reaction, Reactivity of metal complexes, Inert and Labile complexes, substitution reactions in octahedral and square planar complexes and their mechanism, Kinetic application of Valence Bond and Crystal field theories, trans effect and its influence, water exchange, anation and base hydrolysis, stereochemistry, inner and outer sphere electron transfer mechanism, Marcus-Hush Theory.

UNIT 2 **Organometallics:** 18-Electron Rule, Ligands in Organomettallics, Synthesis, bonding and reactions of Metal alkyls, carbenes, carbynes, alkenes, alkynes, and allyl complexes. Hydrides, Metallocenes, Metal arene complexes and Fullerene complexes. Spectral analysis of Organometallic Complexes.

UNIT 3 Homogeneous and heterogeneous catalysis: Stiochiometric reactions for Organometallic catalysts: Dissociation & Substitution, Oxidative addition & carbonylation, Reductive & Hydride elimination, Migratory Insertion and elimination reactions, Displacement and Isomerization reaction.

Hydrogenation, Hydrosilation and Hydrocynation of unsaturated compounds,

Hydroformylation, Wacker (Smidt) Process, Olefin Metathesis, Fischer-Tropsch synthesis, Zeigler-Natta polymerization, Water gas reaction.

UNIT 4 **Magneto chemistry and EPR:** Induction and susceptibility. Lande interval rule, calculation of g-values, Van Vleck's equation and its use. Effect of spin orbit coupling. Magnetic properties of A.E.T terms with reference to Co(I) and Ni(II) complexes. Electron Paramagnetic Resonance Spectroscopy: Hyperfine splitting, Spin orbit coupling, Significance of g-tensor, Zero field splitting, Kramer's degeneracy, Application to inorganic systems.

C. TEXT BOOKS

1. J. E. Huheey, E. A. Keiter and R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity , 4th Ed. Harper Collins (1993).
2. The organometallic Chemistry of transition metals, R.H. Crabtree, John Wiley,1994.

D. BOOKS FOR REFERENCES

1. Advanced Inorganic Chemistry by F. A. Cotton and G. W. Wilkinson, John-Wiley & Sons, 1988, 5th Ed.
2. B. D. Gupta and A. J. Elias; Basic Organometallic Chemistry: Concepts, Synthesis, and Applications, Universities Press (India), 2010.
3. Organometallics by Ch. Elschenbroich, A. Salzer, VCH, 1995, 2nd Ed.
4. Comprehensive Coordination Chemistry eds.: G. Wilkinson, R. D. Gillars and J A McCleverty, Pergamon.

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

CO	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	PSO3	PSO 4
CHE402.1	Learn about the interdisciplinary character of organometallic chemistry among the conventional branches of chemistry as well as the industrial aspects of organometallic chemistry	3		1			2					3
CHE402.2	Understand the chemical processes involved in the various renowned industrial conversions (e.g Olefin polymerization, Hydrogenation, etc.) carried out in presence of organometallic complexes	2			2	1	2	1	2	2	2	1
CHE402.3	Apply knowledge of metal-ligand bond interaction in explaining reactions of metal complexes.	3	1			1	3	1	3	3	3	1
CHE402.4	Apply the concept of Electronic spectroscopy for inorganic compounds analysis.	2	2		1							2

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

PAPER CHE 402: ORGANIC CHEMISTRY IV

Full Mark 100 (80 + 20)

Course objectives: Learn the fundamental ideas of photochemical excitation/deexcitation events, and the molecular events that can intervene at different levels and their applications. The learners should be able to apply, analyze and evaluate the active site structure and functions of some transition metal ion containing enzymes.

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

[CHE402.1]. Learn about Biomolecules: types, structure, functions in cellular life and importance in context with day to day life.

[CHE402.2]. Appreciate the photochemical phenomena by light and be able to design and practically carry out simple photochemical reactions.

[CHE402.3]. Apply photochemistry concepts, plan and program molecules for photochemical application of specific interest

[CHE402.4]. Understand the concept of coenzymes & cofactors, kinetics, mode of action, classification and role in different biological processes

B. SYLLABUS

UNIT-1 Organic Photochemistry – I

Photochemistry of alkenes

Intramolecular reactions of the olefinic bond – geometrical isomerism, cyclization reactions, rearrangement of 1,4– and 1,5– dienes. Photochemistry of Carbonyl Compounds

Intramolecular reactions of carbonyl compounds – saturated, cyclic and acylic, β,ϒ- unsaturated and α,β-unsaturated compounds. Cyclohexadienones.

UNIT-2 Organic Photochemistry – II

Photochemistry of Aromatic Compounds, Isomerisations, additions and substitutions, Miscellaneous Photochemical Reactions, Photo-Fries reactions of anilides. Photo-Fries rearrangement. Barton reaction. Singlet molecular oxygen reactions. Photochemical formation of smog. Photodegradation of polymers. Photochemistry of vision.

UNIT-3 Bioorganic chemistry-I

Example of some typical enzyme mechanism: chymotrypsin, ribonuclease, lysozyme, carboxypeptidase A. Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, Thiamine pyrophosphate, pyridoxal phosphate, NAD+, NaDP+, FMN, FAD, lipoic acid, Vitamin B12

UNIT-4 Bioorganic Chemistry II: Mechanism of reactions catalyzed by cofactors. A Nucleophilic displacement on a phosphorous atom, multiple displacement reaction and coupling of ATP cleavage to endergonic processes, transfer of sulphate, addition and elimination reactions, enolic intermediates in the isomerization reactions, β cleavage and condensation, isomerization, rearrangement, carboxylation, decarboxylation.

TEXT BOOKS

1. Photo Chemistry and Pericyclic Reactions: Jagdamba Singh and Jaya Singh, New Age International.
2. Bioorganic Chemistry, A chemical Approach to Enzyme action, Hermann Dugas and C.Penny Springer Verlag

Reference Books:

1. Fundamentals of Photochemistry, K.K. Rohtagi- Mukherjee, Wiley-Eastern
2. Organic Photochemistry, A.Cox and T Camp,McGraw-Hill
3. Photochemistry by R.P. Kundall and A. Gilbert. Thomson Nelson.
4. Enzyme Chemistry : Impact and Applications, Ed Collin J. Suckling,Chapman and Hall
5. Enzyme Mechanisms Ed,M.I.page and Williams Royal Society of Chemistry
6. Understanding Enzymes,Trevor Palmer, Prentice Hall

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

CO	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	PSO3	PSO 4
CHE402.1	Biomolecules: types, structure, functions in cellular life and importance in context with day to day life.	3	1	1			2					2
CHE402.2	Appreciate the photochemical phenomena by light and be able to design and practically carry out simple photochemical reactions.	2	2	2		1	2	1	2		2	1
CHE402.3	Apply photochemistry concepts, plan and program molecules for photochemical application of specific interest	2		2			2	1	3	2	3	2
CHE402.4	Understand the concept of coenzymes & cofactors, kinetics, mode of action, classification and role in different biological processes	2			1		2			3		3

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

PAPER CHE 403: PHYSICAL CHEMISTRY III

Full Mark 100 (80 + 20)

Course objectives: To introduce the basic concepts of surface and interfacial chemistry. The subject is very diverse and interdisciplinary in nature. The topics cover the chemical processes that occur at solid-liquid, solid-gas and liquid-gas interfaces. The spectroscopy and microscopy methods to study the interfacial phenomena are also included in the syllabus for the benefit of chemistry, physics, engineering, and biology students.

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

[CHE403.1]. Defines phase, equilibrium, component, degree of freedom and phase rule concepts. Applies these concepts to the field of Materials Science and Engineering

[CHE403.2]. Predict the course of an organic photochemical reaction and identify the product with the type of functional group present on the molecule

[CHE403.3]. Apply photochemistry concepts, plan and program molecules for photochemical application of specific interest

[CHE403.4]. Learn surface active agents, micelles, micro-emulsions, reverse micelle, lipids, liposome and Appreciate micellization process

B. SYLLABUS

UNIT 1 **Phase Rule:** Fundamental concept of phase, component, degrees of freedom, Phase Rule, one component system (water, sulphur system), condense phase rule, two component system (Lead-Silver, Iron- Carbon system), Three Component Systems of both Solids and Liquids, Application and limitation of Phase rule.

UNIT 2 Surface chemistry and Adsorption: Surface Tension, Capillary Action, Adsorption, Types of Adsorption, Physisorption, Chemisorption, Gibbs Adsorption Isotherm, Freundlich's Adsorption Isotherm, Langmuir's Adsorption Isotherm, BET Adsorption Isotherm and its Applications, Heat of Adsorption, Estimation of Surface Areas of Solids from Solution Adsorption Studies.

UNIT 3 **Photochemistry:** Light matter interaction, Laws of photochemistry, Radiative and non-radiative decays, Absorption, Fluorescence, Phosphorescence, delayed fluorescence, Jablonski diagram, Kasha's rule, Concept of quantum yield, Quenching of fluorescence, Derivation of Stern-Volmer equation, Theory of Static and Dynamic quenching, Concept of Fluorescence lifetime and fluorescence anisotropy, Theory of Energy Transfer for a Donor–Acceptor Pair, Distance Measurements Using FRET, Chemiluminescence.

UNIT 4 **Biophysical:** Surface Active Agents, Classification of Surface Active Agents, Concepts on Micelle, Micellization, Critical Micellar Concentration (CMC), Kraft Temperature, Factors Affecting the CMC of Surfactants, Reverse Micelles, Microemulsion, Enzyme kinetics, michaelis menten and lineweaver-burk plots, Nucleosides and nucleotides, Concept of lipids and liposome.

C. TEXT BOOKS

1. Kapoor K. L., Text Book of Physical Chemistry, McGraw Hill, 3rd Edn. 2017
2. G.A. Somorjai, Y. Li , Introduction to Surface Chemistry and Catalysis, 2nd edition, 2010

D. BOOKS FOR REFERENCES

1. Introduction to Surface Chemistry and Catalysis by Gábor A. Somorjai (John Wiley & Sons)
2. Physical Chemistry of Macromolecules by C. Tanford
3. Molecular Photochemistry by N. J. Turro,
4. Principles of Photochemistry by J.A. Baltrop & J.D. Coyle

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

CO	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	PSO3	PSO 4
CHE403.1	Defines phase, equilibrium, component, degree of freedom and phase rule concepts. Applies these concepts to the field of Materials Science and Engineering	3	1	1			2	1	1			2
CHE403.2	Predict the course of an organic photochemical reaction and identify the product with the type of functional group present on the molecule	1	2	1		1	2	1	2		2	1
CHE403.3	Apply photochemistry concepts, plan and program molecules for photochemical application of specific interest	1	2			2		1		1	3	2
CHE403.4	Learn surface active agents, micelles, micro-emulsions, reverse micelle, lipids, liposome and Appreciate micellization process	3	2		1	2						3

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

PAPER CHE 404: PHYSICAL CHEMISTRY IV
Full Mark 100 (80 + 20)

Course Objectives: The learners should be able to apply principles and laws of equilibrium thermodynamics to multicomponent systems. In addition, they should be able to use spectroscopic data to calculate thermodynamic properties of ideal gases, real gases, solids and metals using the principles and techniques of statistical thermodynamics.

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

[CHE103.1]. Learn about binary solutions and partial molar properties.

[CHE103.2]. Calculate change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential. Identify factors affecting equilibrium constant

[CHE103.3]. Acquire the skill to apply thermodynamic concepts in non-equilibrium thermodynamics.

[CHE103.4]. Solve problems based on Debye-Huckel limiting law. Calculate excess thermodynamic properties

[CHE103.5]. Discuss the statistical thermodynamics.

C. SYLLABUS

UNIT 1 **Thermodynamics I:** Brief resume of concepts of laws of thermodynamics. The concept of chemical potential and partial molar properties with their significance. Second law of thermodynamics, Heat engines, and refrigeration engines, entropy, free energy, variation of entropy with temperature, pressure and volume. Change in thermodynamic functions in mixing of ideal gases ($\Delta G_{mix,}$ $\Delta S_{mix,}$ $\Delta V_{mix,}$ ΔH_{mix}**).** Entropy and heat capacities relationships, Gibb's Helmholtz equation and its application.

UNIT 2 **Thermodynamics II:** Third law of thermodynamics, its application to solids, liquids and gases, Nernst heat theorem and its applications. Determination of these quantities. Concept of fugacity and determination of fugacity. Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients, ionic strength.

UNIT 3 **Thermodynamics III:** Non-Equilibrium Thermodynamics, Thermodynamic criteria for non-equilibrium states, entropy production and entropy flow, entropy balance equations for different irreversible processes (e.g., heat flow, chemical reaction etc.) transformations of the generalized fluxes and forces, non-equilibrium stationary states, phenomenological equations, microscopic reversibility and Onsager's reciprocal relations.

UNIT 4 **Statistical Thermodynamics:** Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers) Partition functions-translational, rotational, vibrational and electronic partition functions, calculation of thermodynamic properties in terms of partition function. Fermi-Dirac statistics, distribution law and application to metal. Bose-Einstein statistics - distribution law and application to helium.

D. TEXT BOOKS

1. Physical Chemistry, P.W. Atkins and J. D. Paulo, Oxford, 10th edition New Delhi.
2. Molecular Thermodynamics, D. A. McQuarrie and J. D. Simon. Viva, 1st edition, New Delhi.

E. BOOKS FOR REFERENCES

1. Thermodynamics, G. N. Lewis and M. Randall, McGraw Hill, 2nd edition, New York.

2. Non Equilibrium Thermodynamics, S.R. deGroot and Mazur, Dover, New York.
3. Statistical Mechanics and Thermodynamics, C. Garrod, Oxford Univ. Press, New York.
4. Introduction to thermodynamics of irreversible processes, I. Prigogine, 2nd edition, Interscience,

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

CO	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAM SPECIFIC OUTCOMES			
		PO 1	PO 2	PO 3	PO 4	PO 5	PO 6	PO 7	PSO 1	PSO 2	PSO3	PSO 4
CHE103.1	Learn about binary solutions and partial molar properties.	2	2		3		1	2	2	1		2
CHE103.2	Calculate change in thermodynamic properties, equilibrium constants, partial molar quantities, chemical potential. Identify factors affecting equilibrium constant	3	1		2		1	2		1		2
CHE103.3	Acquire the skill to apply thermodynamic concepts in non-equilibrium thermodynamics.	2	2					1				3
CHE103.4	Solve problems based on Debye-Huckel limiting law. Calculate excess thermodynamic properties	2	2					1	2			2
CHE103.5	Discuss the statistical thermodynamics.	3	1	1				1	1			1

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

PAPER CHE 405: PROJECT AND SEMINAR
Full Mark (80 +20)

The dissertation shall comprise of conducting a small project under faculty members of the department. The title and execution of the project work shall be decided in consultation with the faculty members of the School by a committee constituting HOD and other senior faculty members. The committee may also extend the provision of co-opting the external guide as per the provision provided by the Gangadhar Meher University.

In general, the student is expected to do literature survey in the assigned topic, and to do some kind of experimental investigation, and result analysis. However, final decision regarding the execution of project work rests with the supervisor/co-supervisor and the committee on mutual discussion to the best benefit of the student for academic career. The guideline provided by UGC shall be also considered in this regard.