COURSES OF STUDIES

FOR UNDER 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

U.G. PROGRAM ARTICULATION MATRIX

SEMESTER	COURCE CODE	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PSO 1	PSO 2	PSO3	PSO 4
I	CHE DMT 101 & CHE IDMT 103	2	2	2	1	0	1	2	2	1	0	2
	CHE DMP 107 & CHE IDMP 108	2	2	2	1	0	1	2	2	1	0	2
	CHE DMI 102 & CHE IDMI 104	2	2	0	1	0	1	1	2	1	2	2
	CHE VOT 105	3	2	2	1	1	2	0	3	2	0	3
	CHE VOT 106	3	0	1	3	1	3	3	3	3	3	3
II	CHE DMT 201 & CHE IDMT 203	3	2	1	2	1	3	2	3	2	3	3
	CHE DMP 207 & CHE IDMP 208	3	2	3	1	1	2	2	3	1	0	2
	CHE DMI 202 & CHE IDMI 204	3	2	0	3	0	2	1	3	3	3	3
	CHE VOT 205	3	2	0	1	0	2	3	3	2	0	3
	CHE VOP 206	3	0	2	2	2	0	0	1	3	3	1
III	CHE DMT 301 & CHE IDMT 303	3	2	1	3	1	2	3	3	0	2	3
	CHE DMP 307 & CHE IDMP 308	3	2	2	1	2	3	3	3	0	0	3
	CHE DMI 302 & CHE IDMI 304	2	2	0	1	0	1	2	2	1	2	2
	CHE VOT 305	3	2	0	0	0	2	3	3	2	0	3
	CHE VOP 306	3	0	2	1	2	2	3	3	2	3	3
IV	CHE DMT 401& CHE IDMT 403	3	2	1	3	1	2	3	3	0	2	3
	CHE DMP 407 & CHE IDMP 408	3	2	2	1	2	3	3	3	0	0	3
	CHE DMI 402 & CHE IDMI 404	2	2	0	1	0	1	2	2	1	2	2
	CHE VOT 405	3	2	0	0	0	2	3	3	2	0	3
	CHE VOP 406	3	0	2	1	2	2	3	3	2	3	3
V	CHE DMT 501 & CHE IDMT 503	3	2	1	3	1	2	3	3	0	2	3
	CHE DMP 507 & CHE IDMP 508	3	2	2	1	2	3	3	3	0	0	3
	CHE DMT(I) 505	2	2	0	1	0	1	2	2	1	2	2
	CHE DMP(I) 509	3	2	0	0	0	2	3	3	2	0	3
	CHE DMI 502 &	3	0	2	1	2	2	3	3	2	3	3

	CHE IDMI 504											
VI	CHE DMT 601 & CHE IDMT 604	3	2	1	3	1	2	3	3	0	2	3
	CHE DMP 607 & CHE IDMP 608	3	2	2	1	2	3	3	3	0	0	3
	CHE DMT 603 / CHE IDMT 606	2	2	0	1	0	1	2	2	1	2	2
	CHE DMI 602 & CHE IDMI 605	3	2	0	0	0	2	3	3	2	0	3
VII	CHE DMT 701	2	2	2	1	0	1	2	2	1	0	2
	CHE DMP 705	2	2	2	1	0	1	2	2	1	0	2
	CHE DMP 706	2	2	0	1	0	1	1	2	1	2	2
	CHE DMT 703	3	2	2	1	1	2	0	3	2	0	3
	CHE DMT(I) 704	3	0	1	3	1	3	3	3	3	3	3
	CHE DMP(I) 707	3	2	1	3	1	2	3	3	0	2	3
VIII	CHE D 801	3	2	2	1	2	3	3	3	0	0	3
	CHE D 801A	2	2	0	1	0	1	2	2	1	2	2
	CHE D 801B	3	2	0	0	0	2	3	3	2	0	3
	CHE D 801C	3	0	2	1	2	2	3	3	2	3	3
	CHE D 801D	2	1	1	3	2	1	3	3	2	0	3
IX	CHE DMT 901	3	2	1	3	1	2	3	3	0	2	3
	CHE DMP 905	3	2	2	1	2	3	3	3	0	0	3
	CHE DMT 902	2	2	0	1	0	1	2	2	1	2	2
	CHE DMP 906	3	2	0	0	0	2	3	3	2	0	3
	CHE DMT 903	3	0	2	1	2	2	3	3	2	3	3
	CHE DET 904	2	1	1	3	2	1	3	3	2	0	3
X	CHE DMT 1001	3	2	1	3	1	2	3	3	0	2	3
	CHE DMT 1002	3	2	2	1	2	3	3	3	0	0	3
	CHE DMT 1003	2	2	0	1	0	1	2	2	1	2	2
	CHE DET 1004A /1004B	3	2	0	0	0	2	3	3	2	0	3
	CHE DMP 1005	3	0	2	1	2	2	3	3	2	3	3
	CHE DMP1006A /1006B	3	2	0	0	0	2	3	3	2	0	3
AVERAGE		2.65	1.54	1.05	1.51	1.02	1.77	2.45	2.71	1.34	1.2	2.68

UNDER GRADUATE PROGRAMME STRUCTURE DEPARTMENT OF CHEMISTRY

Post graduate program comprising two years, will be divided into 10 (ten) semesters each of six months duration.

Year	Semesters	
First Year	Semester I	Semester II
Second Year	Semester III	Semester IV
Third Year	Semester V	Semester VI
Fourth Year (**UG Hons.)**	Semester VI	Semester VIII
Fifth Year	Semester IX	Semester X

Course Structure for B. Sc. and (UG Hons./PG Programme)							
CHEMISTRY							
1 credit = 1 hour per week for Theory and 2 hours per week for Laboratory							
Course Structure	**Course Code**	**Course Name**	**Marks**		**Total Marks**	**Duration (Hrs) of Exam (End Term**	**Credit**
			END TERM	**MID TERM**			
SEMESTER-I							
Value Added/Ability Enhancement Compulsory Course – I	**ENG VB 100**	English Communications (Offered by Respective Department/University Level)					
Disciplinary & Inter-disciplinary Major – I	**CHE DMT 101 & CHE IDMT 103**	Atomic Structure, Chemical Bonding, Fundamentals, Stereochemistry and Hydrocarbons	**60**	**40**	**100**	**3**	**4+4**
	CHE DMP 107 & CHE IDMP 108	Inorganic Chemistry Practical - I	**--**	**--**	**50**	**2**	**2+2**
Disciplinary & Inter-disciplinary Minor – I	**CHE DMI 102 & CHE IDMI 104**	States of Matter and Colloidal State	**30**	**20**	**50**	**2**	**2+2**
Vocational	**CHE VOT**	Basic Concepts of	**30**	**20**	**50**	**2**	**2**

Course – I (Skill Enhancement Course)	**105**	Physical Chemistry Experiments, Energy, and Environment					
	CHE VOT 106	Vocational Chemistry Practical – I	**30**	**20**	**50**	**2**	**2**
							20
SEMESTER-II							
Value Added/Ability Enhancement Compulsory Course – II	**CSC VB 200**	Computer Studies (Offered by Respective Department/University Level)					
Disciplinary & Inter-disciplinary Major – II	**CHE DMT 201 & CHE IDMT 203**	Thermodynamics – I, Ionic Equilibria & Conductance, Periodicity, Acid-Bases, & Radioactivity	**60**	**40**	**100**	**3**	**4+4**
	CHE DMP 207 & CHE IDMP 208	Physical Chemistry Practical - I	**--**	**--**	**50**	**2**	**2+2**
Disciplinary & Inter-disciplinary Minor – II	**CHE DMI 202 & CHE IDMI 204**	Chemistry in Daily Life	**30**	**20**	**50**	**2**	**2+2**
Vocational Course – II (Skill Enhancement Course)	**CHE VOT 205**	Cosmetics, Perfumes, & Pharmaceutical Chemistry	**30**	**20**	**50**	**2**	**2**
	CHE VOP 206	Vocational Chemistry Practical – II/ Internship (Industrial Visit)	**30**	**20**	**50**	**2**	**2**
							20
SEMESTER-III							
Value Added/Ability Enhancement Compulsory Course – III	**EVS VB 300**	Environmental Studies (Offered by Respective Department/University Level)	-				
Disciplinary & Inter-disciplinary Major – III	**CHE DMT 301 & CHE IDMT 303**	Substitution, Elimination Reactions, Carbonyl Chemistry, Thermodynamics – II, Electrochemistry & Chemical Kinetics	**60**	**40**	**100**	**3**	**4+4**
	CHE DMP 307 & CHE IDMP 308	Organic Chemistry Practical – I	**--**	**--**	**50**	**2**	**2+2**
Disciplinary &	**CHE DMI**	Basic Analytical	**30**	**20**	**50**	**2**	**2+2**

Inter-disciplinary Minor – III	**302 & CHE IDMI 304**	Chemistry					
Vocational Course – III (Skill Enhancement Course)	**CHE VOT 305**	Cement & Ores, Pesticides & Fuel	**30**	**20**	**50**	**2**	**2**
	CHE VOP 306	Vocational Chemistry Practical – III /Industrial Visit	**30**	**20**	**50**	**2**	**2**
							20
SEMESTER – IV							
Value Added/Ability Enhancement Compulsory Course – III	**DMM VB 400**	Disaster Management (Offered by Respective Department/University Level)	**-**				
Disciplinary & Inter-disciplinary Major – IV	**CHE DMT 401 & CHE IDMT 403**	Chemistry of *-s, -p, -d and -f* Block elements, Rearrangement and Reagents in Organic Chemistry	**60**	**40**	**100**	**3**	**4+4**
	CHE DMP 407 & CHE IDMP 408	Physical Chemistry Practical – II	**--**	**--**	**50**	**2**	**2+2**
Disciplinary & Inter-disciplinary Minor – IV	**CHE DMI 402 & CHE IDMI 404**	Chemical and Phase Equilibria, Solutions and Colligative Properties	**30**	**20**	**50**	**2**	**2+2**
Vocational Course – II (Skill Enhancement Course) CHM P 223	**CHE VOT 405**	Techniques of Instrumental Analysis	**30**	**20**	**50**	**2**	**2**
	CHE VOP 406	Hands Training on Instruments	**30**	**20**	**50**	**2**	**2**
							20
SEMESTER-V							
Value Added/Ability Enhancement Compulsory Course – III	**VB 500**	Creative Expression – I (Offered by Respective Department/University Level)	**-**				
Disciplinary Major – V	**CHE DMT 501 & CHE IDMT**	Photochemistry, Catalysis, Quantum Chemistry & Spectroscopy	**60**	**40**	**100**	**3**	**4+4**

	503						
	CHE DMP 507 & CHE IDMP 508	Physical Chemistry Practical - III	**--**	**--**	**50**	**2**	**2+2**
Disciplinary Major (Internship)	**CHE DMT(I) 505**	Chemistry Research Orientation	**30**	**20**	**50**	**2**	**2**
	CHE DMP(I) 509	Organic Chemistry Practical - II	**30**	**20**	**50**	**2**	**2**
Disciplinary Minor – V	**CHE DMI 502 & CHE IDMI 504**	Advanced Analytical Chemistry	**30**	**20**	**50**	**2**	**2+2**
							20
SEMESTER-VI							
Value Added/Ability Enhancement Compulsory Course – III	**VB 600**	Creative Expression – II (Offered by Respective Department/University Level)	**-**				
Disciplinary & Inter-disciplinary Major – VI	**CHE DMT 601 & CHE IDMT 604**	Coordination & Organometallics Chemistry	**60**	**40**	**100**	**3**	**4+4**
	CHE DMP 607 & CHE IDMP 608	Inorganic Chemistry Practical – II	**--**	**--**	**50**	**2**	**2+2**
	CHE DMT 603 / CHE IDMT 606	Bioorganic Chemistry	**60**	**40**	**100**	**2**	**4**
Disciplinary & Inter-disciplinary Minor – VI	**CHE DMI 602 & CHE IDMI 605**	Organic Spectroscopy	**30**	**20**	**50**	**2**	**2+2**
			30	**20**	**50**		**20**
SEMESTER-VII							
Disciplinary Major	**CHE DMT 701**	Transition and Inner Transition Metal	**60**	**40**	**100**	**3**	**4**

(UG Hons./PG Programme)		Chemistry					
	CHE DMP 705	Inorganic Chemistry Practical - III	**--**	**--**	**50**	**2**	**2**
	CHE DMT 702	Organic Reaction Mechanism and Stereochemistry	**60**	**40**	**100**	**3**	**4**
	CHE DMP 706	Organic Chemistry Practical - III	**30**	**20**	**50**	**2**	**2**
	CHE DMT 703	Thermodynamics, Catalysis-, Electro- & Surface Chemistry	**60**	**40**	**100**	**3**	**4**
	CHE DMT(I) 704	Research methodology for Chemistry	**30**	**20**	**50**	**2**	**2**
	CHE DMP(I) 707	Chemistry software uses for research	**30**	**20**	**50**	**2**	**2**
							20
SEMESTER-VIII							
Disciplinary Major **(UG Hons./PG Programme)**	**CHE D 801**	**D 801: Project/Dissertation**					**20**
	CHE D 801A	• D 801A: Development of project/ Research proposal/Lab Work	**--**	**--**	**100**	**3**	**4**
	CHE D 801B	• D 801B: Pre-Submission presentation/Data collection	**--**	**--**	**100**	**3**	**4**
	CHE D 801C	• D 801C: Report Writing/Write-up/ Dissertation Report	**--**	**--**	**200**		**8**
	CHE D 801D	• D 801D: Presentation &Viva Voce	**--**	**--**	**100**		**4**
		•					**20**
SEMESTER – IX							
Disciplinary Major **(PG Programme)**	**CHE DMT 901**	Organometallic Chemistry	**60**	**40**	**100**	**3**	**4**
	CHE DMP 905	Inorganic Chemistry Practical – IV	**--**	**--**	**50**	**2**	**2**
	CHE DMT 902	Principle of Organic Synthesis and Organic Spectroscopy	**60**	**40**	**100**	**3**	**4**
	CHE DMP 906	Organic Chemistry Practical – IV	**30**	**20**	**50**	**2**	**2**
	CHE DMT 903	Quantum-, Statistical-Mechanics, & Chemical Kinetics	**60**	**40**	**100**	**3**	**4**

	CHE DET 904	Molecular Spectroscopy	**60**	**40**	**100**	**3**	**4**
							20
SEMESTER – X							
Disciplinary Major **(PG Final Year)**	**CHE DMT 1001**	Bio-Inorganic & Sensor Materials Chemistry	**60**	**40**	**100**	**3**	**4**
	CHE DMT 1002	Pericyclic Reaction, Photochemistry and Free Radical Chemistry	**60**	**40**	**100**	**3**	**4**
	CHE DMT 1003	Chemical Bonding, Group Theory and Solid State Chemistry	**60**	**40**	**100**	**3**	**4**
	CHE DET 1004A /1004B	Discipline Specific Elective Paper – I (opt any one course from DET offered by Dept. Of Chemistry)	**60**	**40**	**100**	**3**	**4**
	CHE DMP 1005	Physical Chemistry Practical – IV	**--**	**--**	**50**	**2**	**2**
	CHE DMP1006A /1006B	Nanomaterials Chemistry Practical/ Advanced Heterocyclic Chemistry Practical (2)	**--**	**--**	**50**	**2**	**2**
							20
		Grand Total					**200**

*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.

Minor Paper in Chemistry							
Semester	**Course Code**	**Course Name**	**Marks**		**Total Marks**	**Duration (Hrs) of Exam (End Term**	**Credit**
			END TERM	**MID TERM**			
I	**CHE DMI 102 & CHE IDMI 104**	States of Matter and Colloidal State	**30**	**20**	**50**	**2**	**2**
II	**CHE DMI 202 & CHE IDMI 204**	Chemistry in Daily Life	**30**	**20**	**50**	**2**	**2**
III	**CHE DMI 302 & CHE IDMI 304**	Basic Analytical Chemistry	**30**	**20**	**50**	**2**	**2**
IV	**CHE DMI 402 & CHE IDMI 404**	Chemical and Phase Equilibria, Solutions and Colligative Properties	**30**	**20**	**50**	**2**	**2**
V	**CHE DMI 502 & CHE IDMI 504**	Advanced Analytical Chemistry	**30**	**20**	**50**	**2**	**2**
VI	**CHE DMI 602 & CHE IDMI 605**	Organic Spectroscopy	**30**	**20**	**50**	**2**	**2**

The I-VI Minor disciplinary/multidisciplinary paper may be substituted by the following additional Minor papers subject to the availability of the Teacher and class load of the discipline/teacher in any semester.

Additional Course:

CHE DMI 102/ CHE IDMI 104: IT Skill for Chemist
CHE DMI 202/ CHE IDMI 204: Green Methods in Chemistry
CHE DMI 302/ CHE IDMI 304: Basic of Nanomaterials
CHE DMI 402/ CHE IDMI 404: Crystalline Materials and Properties
CHE DMI 502/ CHE IDMI 504: Inorganic Materials of Industrial Importance
CHE DMI 602/ CHE IDMI 605: Basic of Drug Design & Medicinal Chemistry

Minor Paper in Chemistry							
Semester	Course Code	Course Name	Marks		Total Marks	Duration (Hrs) of Exam (End Term	Credit
			END TERM	MID TERM			
I	CHE VOT 105	Basic Concepts of Physical Chemistry Experiments, Energy, and Environment	30	20	50	2	2
I	CHE VOP 106	Vocational Chemistry Practical – I	30	20	50	2	2
II	CHE VOT 205	Cosmetics, Perfumes, & Pharmaceutical Chemistry	30	20	50	2	2
II	CHE VOP(I) 206	Vocational Chemistry Practical – II /Internship (Industrial visit)	30	20	50	2	2
II	CHE VOT 305	Cement, Extraction of Ores, Pesticides & Fuel Chemistry	30	20	50	2	2
III	CHE VOP 306	Vocational Chemistry Practical – III	30	20	50	2	2
IV	CHE VOT 405	Techniques of Instrumental Analysis (Principles and Applications of X-ray diffraction, FT-IR, UV, GCMS, LCMS etc.)	30	20	50	2	2
IV	CHE VOP (I) 406	Hands Training on Instruments	30	20	50	2	2

Discipline Specific Elective Course* (Opt any one)				
Course Code	Course Structure	Title of Paper	Marks	Credit
CHE DET 904	Elective	Molecular Spectroscopy	100	04
CHE DET1004A	Elective	Introduction to Nanomaterials & Nanotechnology	100	04
CHE DET1004B	Elective	Advanced Heterocyclic Chemistry	100	04

SEMESTER – I

PAPER CODE: CHE DMT 101/CHE IDMT 103: Atomic Structure, Chemical Bonding, Fundamentals, Stereochemistry and Hydrocarbons

Full Mark 100 (60 + 40)

Course Objectives: The learners should be able to: In Part A: Learn the basics of atomic structure & chemical bonding and redox reactions. In Part B: Understanding the fundamentals, stereochemistry and hydrocarbons.

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

PART-A:

[CHE DMT 101/CHE IDMT 103.1]. Recall basic concepts of atomic structure, schrödinger's wave equation and pauli's exclusion principle.
[CHE DMT 101/CHE IDMT 103.2]. Learn the classifications of bonds and general characteristics.
[CHE DMT 101/CHE IDMT 103.3]. Learn the basics of redox reactions, precipitation and complex formation and redox titrations.

PART-B:

[CHE DMT 101/CHE IDMT 103.1]. Learn the basics of structure, reactivity, mechanism and kinetics of organic reactions.
[CHE DMT 101/CHE IDMT 103.2]. Learn the basics and various types of acids and bases (Lewis acid, Bronsted acids).
[CHE DMT 101/CHE IDMT 103.3]. Understand the basics of stereochemistry, isomerism and stereospecific and stereo selective reactions.

B. SYLLABUS

Part-A

Inorganic Chemistry– I: Atomic Structure & Chemical Bonding,

Unit –I: Atomic Structure

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Types of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals. Contour boundary and probability diagrams.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Unit – II: Chemical Bonding

(i)*Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy

(ii) *Covalent bond:* Lewis structure, Valence Bond theory (Heitler-London approach). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond

lengths. Energetics of hybridization. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, and their ions; HCl, BeF_2, CO_2, (idea of s-p mixing and orbital interaction to be given).

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) *Metallic Bond & Weak Chemical Forces:* Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids, van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Repulsive forces, Hydrogen bonding, effects of chemical force, melting and boiling points, solubility energetics of dissolution process.

Unit – III: Redox

Redox equations, Standard electrode potentials, redox potentials and formal potentials, Nernst equation, redox potentials to explore the feasibility of reaction and calculation of values of equilibrium constant, redox potential as a function of pH, precipitation and complex formation, redox titrations and redox indicators, Frost and Latimer diagrams of redox potentials. Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell.

Reference Books:

1. Lee, J.D. Concise Inorganic Chemistry, ELBS, 1991.
2. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, Oxford, 1970
3. Atkins, P.W. & Paula, J. Physical Chemistry, Oxford Press, 2006.
4. Day, M.C. and Selbin, J. Theoretical Inorganic Chemistry, ACS Publications 1962.
5. Wahid U. Malic, G. D. Tuli, R. D. Madan, Inorganic Chemistry, S. Chand & Co. Ltd
6. R. Sarkar and N. Saha, General & Inorganic Chemistry, New Central Book Agency
7. Puri, Sharma and Kalia, Principle of Inorganic Chemistry, Milestone publishers & distributors

Part B

Organic Chemistry – I : Fundamentals, Stereochemistry and Hydrocarbons

Unit I: Structure, Reactivity and Mechanism

Atomic orbitals, Hybridization, Bonding in Carbon Compounds, The breaking and forming of bonds, Factors Influencing Electron availability, Steric factors, Reagents types and Reaction types. Kinetics of reaction and Investigation of Reaction Mechanism.

Unit II: The strength of acids and bases

Definition, Various types of acids and bases (Lewis acid, Bronsted acids). The origin of acidity and basicity in organic compounds, The strength of acids and bases with comparative study.

Unit III: Basics of Stereochemistry

Chirality, Configuration and conformation, Geometrical isomerism, Optical isomerism, Enantiomers, Diastereomers, projection formulae, D-L and R-S nomenclature (CIP rules), Erythro and threo nomenclature. dl- and meso compounds, Atropisomerism, Stereospecific and stereoselective reactions,

Conformations vs reactivity of cycloalkanes.

Unit IV: Hydrocarbons and Their Functional Groups

Alkenes and alkynes: Synthesis through elimination, electrophilic addition reactions: addition of halogens, hydrogen halides, water, oxymercuration-demercuration, addition of borane; hydrogenation, oxidation, ozonolysis.

Alkyne synthesis, addition of halogen, hydrogen halide, water, boranes, hydrogenation, acetylide ion

Aromaticity, antiaromaticity, Electrophilic aromatic substitution: nitration, halogenation, sulfonation, Friedel-Crafts alkylation and acylation reactions, reactions of substituted benzene: electronic effect of substituents, important reactions of phenols, thiols, aromatic amino compounds and naphthalene. Nucleophilic aromatic substitution: substitution of hydrogen, substitution of atoms other than hydrogen, substitution via aryne intermediates.

C. Reference Books:

1. A Guidebook to Mechanism in Organic Chemistry-By Peter Sykes
2. Organic Chemistry (2nd Edition)-By Jonathan Clayden, Nick Greeves and Stuart warren
3. Organic Chemistry (3rd Edition)-By David Klein
4. Organic Chemistry (8th Edition)-By Paula Yurkanis Bruice

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
PART-A: [CHE DMT 101/CHE IDMT 103.1	Recall basic concepts of atomic structure, schrödinger's wave equation and pauli's exclusion principle.	3		2				2	2			2
[CHE DMT 101/CHE IDMT 103.2	Learn the classifications of bonds and general characteristics.	2	2				2		2	1		1
[CHE DMT 101/CHE IDMT 103.3	Learn the basics of redox reactions, precipitation and complex formation and redox titrations.	1			2		2				3	2
PART-B: [CHE DMT 101/CHE IDMT 103.1	Learn the basics of structure, reactivity, mechanism and kinetics of organic reactions.	2		1			2			2	2	2
[CHE DMT 101/CHE IDMT 103.2	Learn the basics and various types of acids and bases (Lewis acid, Bronsted acids).	2		1		3		2	2			3
[CHE DMT 101/CHE IDMT 103.3	Understand the basics of stereochemistry, isomerism and stereospecific and stereo selective reactions.											

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

CHE DMP 107/CHE IDMP 108: Inorganic Chemistry Practical – I

A. SYLLABUS

(A) Titrimetric Analysis

(i) Calibration and use of apparatus
(ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

(i) Estimation of carbonate and hydroxide present together in mixture.
(ii) Estimation of carbonate and bicarbonate present together in a mixture.
(iii) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

(i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution.
(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
(iii) Estimation of Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

OR

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

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

B. Reference text:

1. Vogel, A.I. A Textbook of Quantitative Inorganic Analysis, ELBS.
2. Ghosal, Mahapatra and Nad, An Advanced Course in Practical Chemistry

SEMESTER – II

PAPER CODE: CHE DMT 201/CHE IDMT 203: Thermodynamics – I, Ionic Equilibria, Conductance, Periodicity, Acid-Bases & Radioactivity

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basic introduction of thermodynamics and thermodynamics laws, thermochemistry, ionic equilibria, conductance and quantitative aspects of Faraday's laws of electrolysis. Understand the basic chemistry of periodicity, acid-bases & radioactivity.

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

PART-A

[CHE DMT 201/CHE IDMT 203.1]. Learn the Introduction of different terms and processes in thermodynamics and laws.

[CHE DMT 201/CHE IDMT 203.2]. Understand ionic equilibria, salt hydrolysis, and theory of acid–base indicators.

[CHE DMT 201/CHE IDMT 203.3]. Learn the ideas on conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes.

PART-B

[CHE DMT 201/CHE IDMT 203.1]. Basics of periodic table and *s, p, d, f* block elements.

[CHE DMT 201/CHE IDMT 203.2]. Learn the lewis acid-base concepts and reactions, and classification of acids and bases as hard and soft.

[CHE DMT 201/CHE IDMT 203.3]. Learn the basic of radioactive and instrumental analysis of radioactive elements.

B. SYLLABUS

Part- A

Physical Chemistry – I: Thermodynamics – I, Ionic Equilibria & Conductance

Unit – I: Thermodynamics – I

Introduction of different terms and processes in thermodynamics: [systems (isolated, closed, open) and surrounding, macroscopic properties (extensive and intensive), kinds of processes], state and path functions and their differentials. Zeroth law of thermodynamics.

First Law: concept of heat, *q*, work, *w*, internal energy, *U*, sign convention for heat and work; statement of first law; enthalpy, *H*; heat capacities (C_v, C_p) and relation between them for ideal gases. Reversible and irreversible processes, maximum work; calculations of *q*, *w*, *U* and *H* for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Ideal gas law for adiabatic reversible expansion, comparison of adiabatic and isothermal reversible expansion. Joule-Thomson effect, Joule-Thomson coefficient in ideal and real (van der Waals) gases, inversion temperature.

Thermochemistry: Standard state, standard enthalpy of formation, Hess's Laws of constant heat summation and its application. Change in internal energy (ΔU) and enthalpy (ΔH) of chemical reactions, relation between ΔU and ΔH, variation of heat of reaction with temperature (Kirchhoff's equation). Enthalpy of neutralization. Bond Energy – Bond dissociation energy and its calculation from thermo-chemical data. Adiabatic flame temperature and explosion temperature.

Unit – II: Ionic Equilibria

Arrhenius theory of electrolytic dissociation: strong, moderate, and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids (exact treatment).

Salt hydrolysis – calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions, derivation of Henderson-Hasselbalch equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Theory of acid–base indicators; selection of indicators and their limitations.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Qualitative treatment of acid – base titration curves (calculation of pH at various stages).

Unit – III: Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes (Kohlrausch square root law). Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry.

Reference Books:

- Atkins, P. W. & Paula, J. de Atkin's: *Physical Chemistry* 10th Ed., Oxford University Press (2006).
- Ball, D. W.: *Physical Chemistry*, Thomson Press, India (2007).
- Castellan, G. W.: *Physical Chemistry* 4th Ed. Narosa (2004).
- Mortimer, R. G. Physical Chemistry 3rd Ed. Elsevier: NOIDA, U.P. (2009).
- Puri, B. R., Sharma L. R., and Pathania M. S.: *Principle of Physical Chemistry*, Eds. 44th, Vishal Publishing Co., Jalandhar, (2010).
- Kotz J. C., Treichel P. M. & Townsend J. R.: *General Chemistry*, Cengage Lening India Pvt. Ltd., New Delhi (2009).

Part - B

Inorganic Chemistry – II: Periodicity, Acid-Bases & Radioactivity

Unit – I: Periodicity

Periodic table and *s*, *p*, *d*, *f* block elements. Detailed discussion of the following properties of the elements,

with reference to *s* & *p*-block.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table, (b) Atomic radii (van der Waals), (c) Ionic and crystal radii, (d) Covalent radii (octahedral and tetrahedral), (e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy. (f) Electron gain enthalpy, trends of electron gain enthalpy. (g) Electronegativity, Pauling's/ Mulliken's/ Alfred-Rochow scales / and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

Unit – II: Acid & Bases

Arrhenius, Brönsted-Lowry, Lux-Flood, Lewis acid-base concepts and reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Factors affecting strengths of Lewis acids and bases, Classification of acids and bases as hard and soft, Pearsons HSAB concept, acid-base strength and hardness and softness, symbiosis, application of HSAB theory.

Non-aqueous solvents

Physical properties of a solvent, types of solvents and their general characteristics, reactions in non-aqueous solvents with reference to liquid NH_3, liquid SO_2 and liquid HF.

Unit – III: Radioactivity

Radioactive decay, half life and average life of radio elements, units of radioactivity, natural radioactive disintegration series, Instrumental analysis of radioactive elements, radioactive equilibrium, group displacement law, isotope, isotone, isobars and nuclear isomerism. Application of isotope in medicine, agriculture, reaction mechanism (isotope as tracer), age of minerals, age of earth, radio carbon dating, nuclear particles, nuclear forces: meson exchange theory.
Nuclear models (elementary idea), nuclear stability, nuclear binding energy, nuclear reactions, magic numbers, mass defect, proton-neutron ratio, packing fraction, Artificial radioactivity, transmutation of elements, fission, fusion and spallation reaction. Nuclear energy, hazards of nuclear radiations and safety measures.

C. Reference Books:

- Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
- Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry 3rd Ed.*, John Wiley Sons, N.Y. 1994.
- Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
- Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 4th Ed.*, Pearson, 2010.
- Shriver & Atkins, *Inorganic Chemistry 5th 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
PART-A CHE DMT 201/CHE IDMT 203.1	Learn the Introduction of different terms and processes in thermodynamics and laws.	2					1	2		1		2
CHE DMT 201/CHE IDMT 203.2	Understand ionic equilibria, salt hydrolysis, and theory of acid–base indicators.	2		3			1	2	2	1		2
CHE DMT 201/CHE IDMT 203.3	Learn the ideas on conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes.	2	2	2	3	1			2			1
PART-B CHE DMT 201/CHE IDMT 203.1	Basics of periodic table and *s*, *p*, *d*, *f* block elements	1	1						2			3
CHE DMT 201/CHE IDMT 203.2	Learn the lewis acid-base concepts and reactions, and classification of acids and bases as hard and soft.	1		3	1			1	1			3
CHE DMT 201/CHE IDMT 203.3	Learn the basic of radioactive and instrumental analysis of radioactive elements.	1		3	1			1	1			3

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

PAPER CODE: CHE DMP 207/CHE IDMP 208: Physical Chemistry Practical – I

Marks: 50

A. SYLLABUS

Thermochemistry:

- Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
- Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- Calculation of the enthalpy of ionization of ethanoic acid.
- Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.
- Determination of basicity/proticity of a poly-protic acid by the thermo-chemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
- Determination of enthalpy of hydration of copper sulfate.
- Study of the solubility of benzoic acid in water and determination of ΔH.

Surface tension measurements:

- Determine the surface tension by (i) drop number.
- Study the variation of surface tension of detergent solutions with concentration.
- Surface tension composition curve for a binary liquid mixture.

Viscosity measurement using Ostwald's viscometer:

- Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
- Study the variation of viscosity of sucrose solution with the concentration of solute.
- Viscosity composition curve for a binary liquid mixture.

pH metry

- Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
- Preparation of buffer solutions of different pH by
  - **(a)** Sodium acetate-acetic acid
  - **(b)** Ammonium chloride-ammonium hydroxide
- pH metric titration of (i) strong acid *versus* strong base, (ii) weak acid *versus* strong base.
- Determination of dissociation constant of a weak acid.
- To study the dissociation constant of amino acid (glycine) and hence the isoelectric point of the acid.

Conductometry:

- Determination of cell constant.

- Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- Perform the following conductometric titrations:
  - **(a)** Strong acid *versus* strong base
  - **(b)** Weak acid *versus* strong base
  - **(c)** Dibasic acid *versus* strong base

Any other experiment carried out in the class if permit.

B. Reference Books:

- J. Elias, *A Collection of Interesting General Chemistry Experiments*, Revised Ed., University Press, **2007**.
- C. W. Garland, J. W. Nibler and D. P. Shoemaker, *Experiments in Physical Chemistry*, 8th Ed., McGraw-Hill, **2003**.
- A. M. Halern and G. C. McBane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd Ed., W. H. Freeman and Company, **2006**.
- P. C. Kamboj, *University Practical Chemistry*, 1st Ed., Vishal Publishing, **2013**.
- S. K. Maity and N. K. Ghosh, *Physical Chemistry Practical*, NCBA, **2015**.
- A. K. Nad, B. Mahapatra and A. Ghoshal, *An Advanced Course in Practical Chemistry*, 3rd Ed., New Central Book Agency, **2014**.
- J. B. Yadav, *Advanced Practical Physical Chemistry*, Krishna Prakashan Media, **2010**.
- B. Viswanathan and P. S. Raghavan, *Practical Physical Chemistry*, Viva Books, **2009**.

SEMESTER – III

PAPER CODE: CHE DMT 301/ CHE IDMT 303
Substitution, Elimination Reactions, Carbonyl Chemistry, Thermodynamics-II, Electrochemistry, and Chemical Kinetics.

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basics of nucleophilic substitution and addition reactions and mechanisms. Apply the thermodynamic laws, free energy functions, electrochemistry and chemical kinetics.

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

PART-A

[CHE DMT 301/CHE IDMT 303.1]. Understand the basics of nucleophilic substitution reactions and its mechanisms.

[CHE DMT 301/CHE IDMT 303.2]. Understand the basics knowledge of elimination reactions and its mechanisms.

[CHE DMT 301/CHE IDMT 303.3]. Understand the basics of nucleophilic addition reactions and its mechanisms.

PART-B

[CHE DMT 301/CHE IDMT 303.1]. Learn the basics of thermodynamic laws and free energy functions.

[CHE DMT 301/CHE IDMT 303.2]. Learn the basic concepts and applications of electrochemistry and its titrations.

[CHE DMT 301/CHE IDMT 303.3]. Learn the basic concepts of chemical kinetics and its reaction pathways.

B. SYLLABUS

Part – A

Organic Chemistry – II: Substitution, Elimination Reactions, and Carbonyl Chemistry

Unit – I: Nucleophilic Substitution Reactions at a Saturated Carbon atom (sp^3 Carbon)

Types of Substitution reactions (S_N1, S_N2, S_Ni), neighboring group participation (NGP), factors affecting various SN-type reactions, Competition between S_N1 and S_N2 reactions, Substitution reactions of alcohols, alkyl halides, reactions with epoxides (regioselectivity on acid and base medium).

Unit – II: Elimination Reaction

1,2-(β-) Elimination, E1 Mechanism, E1cb Mechanism, E2 Mechanism, Elimination vs Substitution, Factors affecting Elimination Reactions, 1,1-(α-)Elimination, Pyrolytic Syn Elimination

Unit – III: Nucleophilic addition to C=O (Carbonyl Chemistry)

Addition Reactions at sp^2 Carbons: Addition of Carbon, Hydrogen, oxygen, sulfur and Nitrogen nucleophiles to Carbonyl Compounds, Wittig reaction, Cannizzaro's reaction, α,β-unsaturated carbonyl compounds-preparation and properties, Michael addition, 1,2 Vs 1,4- addition reaction.

Acidity of α-hydrogen: Keto-enol tautomerism, alkylation, acylation, halogenation, Aldol condensation, Robinson annulation, Perkin's reaction, Claisen condensation, Dieckmann condensation Reaction, Stobbe Condensation Reaction, Bamford-Steven, Shapiro reaction, base-catalyzed halogenations reaction of ketones (haloform reactions,), active methylene compounds and their reactions, Malonic ester (DEM), acetoacetic ester (EAA).

Carboxylic acid and its derivatives (esters, anhydrides, acid halides, amides): Relative Reactivities, Nucleophilic acyl substitution reactions, Synthesis and reactions.

Reference Books:

1. A Guidebook to Mechanism in Organic Chemistry-By Peter Sykes
2. Organic Chemistry (2nd Edition)-By Jonathan Clayden, Nick Greeves and Stuart warren
3. Organic Chemistry (3rd Edition)-By David Klein
4. Organic Chemistry (8th Edition)-By Paula Yurkanis Bruice

Part – B

Physical Chemistry - II: Thermodynamics-II, Electrochemistry, and Chemical Kinetics

Unit – I: Thermodynamics – II

Second Law: Limitation of first Law, spontaneous processes and different statement of second law of thermodynamics, Carnot cycle and its efficiency, Carnot theorem; thermodynamic scale of temperature.

Concept of Entropy: Entropy changes in reversible and irreversible processes and of universe, physical concept of entropy (molecular and statistical interpretation of entropy), Calusius inequality; entropy as a function of *V* & *T*, and *P* & *T*; entropy changes of an ideal gas in different processes, entropy change in mixing of gases.

Free Energy Functions: Free energy and its concept, Gibbs (*G*) and Helmholtz (*A*) free energies as thermodynamic quantities and their relationship; variation of free energy with temperature and pressure. Maxwell's relations, thermodynamic equation of state; criteria for reversible and irreversible processes (spontaneity); Gibbs-Helmholtz equations, its application of the determination of ΔG, ΔH, ΔS of a reversible cell reaction.

Third Law: Variation of entropy with temperature (Nernst heat theorem), statement of third law, the concept of residual entropy. Applications of third law for determination of absolute entropies of liquid and gases.

Unit – II: Electrochemistry

Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Single electrode potential, its measurement and sign convention. Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes (iv) qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). Concentration cells with and without transference, liquid junction potential and its elimination; determination of activity coefficients and transference numbers. Fuel cell (Hydrogen-Oxygen), Commercial Cell (Primary & Secondary cell), dry cell, acid-alkali storage cell & introduction of lithium ion cells.

Unit – III: Chemical Kinetics

The concept of reaction rate, order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws; half-life of a reaction.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, qualitative treatment of the theory of absolute reaction rates.

C. Reference Books:

- P. Atkins, J. d. Paula and K. James, *Physical Chemistry*, 11th Ed., Oxford University Press, **2018**.
- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, 2nd Ed., Oxford University Press, **2007**.
- D. R. Crow, *Principles and Applications of Electrochemistry*, 4th Ed., Blackie Academic & Professional, **1994**.
- T. Engel and P. Reid, *Physical Chemistry*, 3rd Ed., Pearson, **2014**.
- S. Glasstone, *Thermodynamics for Chemists*, Affiliated East-West Press P. Ltd, **2003**.
- S. Glasstone, *An Introduction to Electrochemistry*, Affiliated East-West Press P. Ltd., **2013**.
- K. L. Kapoor, *A Text Book of Physical Chemistry: Thermodynamics and Chemical Equilibrium, Vol. 2*, 5th Ed., MsGraw-Hill, **2015**.
- K. L. Kapoor, *A Text Book of Physical Chemistry: Applications of Thermodynamics, Vol. 3*, 5th Ed., McGraw-Hill, **2015**.
- K. J. Laidler, *Chemical Kinetics*, 3rd Ed., Pearson, **2011**.
- R. P. Rastogi and R. R. Mishra, *An Introduction to Chemical Thermodynamics*, 6th Ed., Viksh Publishing House, **2018**.
- B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Ed., Vishal Publishing Co., **2018**.

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
PART-A CHE DMT 301/CHE IDMT 303.1	Understand the basics of nucleophilic substitution reactions and its mechanisms.	2					1	2		1		2
CHE DMT 301/CHE IDMT 303.2	Understand the basics knowledge of elimination reactions and its mechanisms.	2		3			1	2	2	1		2
CHE DMT 301/CHE IDMT 303.3	Understand the basics of nucleophilic addition reactions and its mechanisms.	2	2	2	3	1			2			1
PART-B CHE DMT 301/CHE IDMT 303.1	Learn the principle and concepts of organic compounds chirality and conformations.	1	1						2			3
CHE DMT 301/CHE IDMT 303.2	Learn the basic concepts and applications of electrochemistry and its titrations.	1		3	1			1	1			3
CHE DMT 301/CHE IDMT 303.3	Learn the basic concepts of chemical kinetics and its reaction pathways.	1		3	1			1	1			3

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

PAPER CODE: CHE DMP 307/CHE IDMP 308: Organic Chemistry Practical – I

Full Mark: 50

A. SYLLABUS

1. Determination of the melting points of known and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
2. Chromatography

    a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography
    b. Separation of a mixture of two sugars by ascending paper chromatography
    c. Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC)

Qualitative Analysis

3. a. Detection of special elements N, S and halogen (X = Cl, Br and I)
    b. Detection of non-nitrogenous Functional groups (alcohols, phenols, carbonyl and carboxylic acid and ester functional groups)
    c. Detection of nitrogenous Functional groups (primary nitro, amine and amide functional groups)

4. Identification of functional groups present in a unknown organic sample (Qualitative analysis of unknown organic compounds containing simple functional groups such as alcohols, carboxylic acids, phenols, carbonyl compounds, nitro, amine and amide groups)

B. Reference Books:

- Ghosal, Mahapatra and Nad, An Advanced Course in Practical Chemistry
- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
- Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).

SEMESTER – IV

PAPER CODE: CHE DMT 401/CHE IDMT 403: Chemistry of -s, -p, -d and -f Block elements, Rearrangement and Reagents in Organic Chemistry

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the general characteristic properties, structure and bonding of -s, -p, -d and -f Block elements and rearrangement and reagents in organic chemistry.

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

PART-A

[CHE DMT 401/CHE IDMT 403.1]. Learn the general characteristic, chemical, structure and bonding properties of -s, -p block elements.

[CHE DMT 401/CHE IDMT 403.2]. Understand the characteristic, chemical and bonding properties of d and -f block elements

[CHE DMT 401/CHE IDMT 403.3]. Learn the chemistry of lanthanides & actinides and electronic, colour, spectral and magnetic properties.

PART-B

[CHE DMT 401/CHE IDMT 403.1]. Able to learn reactive intermediates and name reactions and rearrangements.
[CHE DMT 401/CHE IDMT 403.2]. Learn the oxidizing reagents reactions and rearrangements.
[CHE DMT 401/CHE IDMT 403.3]. Learn the heterogeneous and homogeneous catalytic reduction reactions.

B. SYLLABUS

Part – A

Inorganic Chemistry-III: Chemistry of *-s, -p, -d and -f* Block elements

Unit – I: *-s & p-Block Elements:*

s-Block Elements: General characteristic properties, complexes of alkali metals, comparative study of hydrides, oxides, hydroxides, halides, carbonates and bicarbonates of group I and II, Diagonal relationship, Allotropy and catenation, Biological role of alkali and alkaline earth metals.

p-Block Elements: General characteristic properties, comparative study (including diagonal relationship and inert pair effect) of groups 13-17 (B, C, N, O, F) elements and group trends of compounds like hydrides, oxides, halides, and oxy acids.
Study of the following compounds with emphasis on structure, bonding, preparation, properties and

uses (Inorganic Polymers): Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, fullerenes, silanes, Oxides and oxoacids of nitrogen, Phosphorus and chlorine. Peroxo acids of sulphur, halogens, interhalogen compounds, polyhalide ions, and pseudohalogens.

Unit – II: d-Block and Inert Group 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

Noble Gases: Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF_2, XeF_4 and XeF_6; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2). Molecular shapes of noble gas compounds (VSEPR theory).

Unit – III: f-Block Elements:

Chemistry of Lanthanides & Actinides: **E**lectronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides and actinides (ion-exchange method only), important lanthanide compounds, similarities the later actinides and lanthanides elements.

Reference Books:

- Lee, J.D. *Concise Inorganic Chemistry*, ELBS, 1991.
- Douglas, B.E; Mc Daniel, D.H. & Alexander, J.J. *Concepts & Models of Inorganic Chemistry 3rd Ed.*, John Wiley Sons, N.Y. 1994.
- Greenwood, N.N. & Earnshaw. *Chemistry of the Elements*, Butterworth-Heinemann. 1997.
- Cotton, F.A. & Wilkinson, G. *Advanced Inorganic Chemistry*, Wiley, VCH, 1999.
- Miessler, G. L. & Donald, A. Tarr. *Inorganic Chemistry 4th Ed.*, Pearson, 2010.
- Shriver & Atkins, *Inorganic Chemistry 5th Ed.*

Part – B

Organic Chemistry – III : Rearrangement and Reagents in Organic Chemistry

Unit – I: Rearrangement Reactions

Reactive intermediates and name reactions: Generation, structure, stability and reactions involving the intermediates: Carbocation (Pinacol-Pinacolone Rearrangement, Wagner-Meerwein Rearrangement, Demjanov reaction, Favorski Rearrangement, Fries Rearrangement, Benzil-Benzilic Acid Rearrangement), carbanion (Alkylation, Aldol condensation, Robinson annulation, Claisen condensation, Dieckmann condensation Reaction, Perkin Reaction, Stobbe Condensation Reaction, Bamford-Steven, Shapiro reaction), Free radicals (Allylic halogenations, acyloin condensation, McMurry coupling, Hunsdiecker reaction, Bouveault-Blanc reduction), carbenes (Wolff Rearrangement, Reimer-Tiemann), nitrenes (Hofmann, Beckmann, Curtius, Schmidt, Lossen Rearrangement), arynes, ylides (Wittig Reaction).

Unit – II: Oxidizing reagents

Chromium reagents, manganese reagents, Ruthenium tetroxide, TPAP, Lead tetraacetate, Osmium tetroxide, Hypervalent Iodine reagents [Dess-Martin periodinane (DMP), o-iodoxybenzoicacid

(IBX)], Cerric ammonium nitrate, DDQ, Selenium dioxide, DMSO based oxidizing reagents, Aluminiumalkoxides (Oppenauer Oxidation), peroxyacids (epoxidation and Baeyer-Villiger oxidation of ketones)

Unit – III: Reducing reagents

Heterogeneous Catalytic hydrogenation, Homogeneous Catalytic hydrogenation (Wilkinson's Catalyst), Dissolving metal reduction (Clemmesen Reduction Reaction, Birch Reduction) Reduction with hydride-transfer reagents (Aluminiumalkoxides, Lithium aluminium hydride, sodium borohydride, DIBAL-H, Tinhydrides, Silanes, diimide, Borane and derivatives.

Reference Books:

1. Modern Methods of Organic Synthesis-By Willium Carruthers and Ian Coldham
2. Organic Chemistry (2nd Edition)-By Jonathan Clayden, Nick Greeves and Stuart warren
3. Organic Chemistry (3rd Edition)-By David Klein
4. Organic Chemistry (8th Edition)-By Paula YurkanisBruice

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
PART-A CHE DMT 401/CHE IDMT 403.1	Learn the general characteristic, chemical, structure and bonding properties of -s, -p block elements.	3		2				2	2			2
CHE DMT 401/CHE IDMT 403.2	Understand the characteristic, chemical and bonding properties of d and -f block elements	2	2				2		2	1		1
CHE DMT 401/CHE IDMT 403.3	Learn the chemistry of lanthanides & actinides and electronic, colour, spectral and magnetic properties.	1			2		2				3	2
PART-B CHE DMT 401/CHE IDMT 403.1	Able to learn reactive intermediates and name reactions and rearrangements.	2		1			2			2	2	2
CHE DMT 401/CHE IDMT 403.2	Learn the oxidizing reagents reactions and rearrangements.	2		1		3		2	2			3
CHE DMT 401/CHE IDMT 403.3	Learn the heterogeneous and homogeneous catalytic reduction reactions.	2		1		3		2	2			3

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

PAPER CODE: CHE DMP 407/CHE IDMP 408: Physical Chemistry Practical – II

A. SYLLABUS

Chemical Equilibrium:

- Equilibrium constant of methyl acetate hydrolysis reaction.
- Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.
- Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:
  (a) simple eutectic and **(b)** congruently melting systems
- Distribution of acetic/ benzoic acid between water and cyclohexane.
- Study the equilibrium of at least one of the following reactions by the distribution method:
  (a) $I_2(aq) + I^-(aq) \rightleftharpoons I_3^-(aq)$ and **(b)** $Cu^{2+}(aq) + nNH_3(aq) \rightleftharpoons [Cu(NH_3)_n]^{2+}$

Chemical Kinetics:

- Study the kinetics of the following reactions.
  (a) Initial rate method: Iodide-persulphate reaction.
  (b) Order of reaction of I_2 – acetone – H^+ ion.
  (c) Integrated rate method:
  (d) Acid hydrolysis of methyl acetate with hydrochloric acid
  (e) Saponification of ethyl acetate.
  (f) Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate.

Potentiometry:

- Perform the following potentiometric titrations:
  (a) Strong acid *versus* strong base
  (b) Weak acid *versus* strong base
  (c) Dibasic acid *versus* strong base

B. Reference Books:

- J. Elias, *A Collection of Interesting General Chemistry Experiments*, Revised Ed., University Press, **2007**.
- C. W. Garland, J. W. Nibler and D. P. Shoemaker, *Experiments in Physical Chemistry*, 8th Ed., McGraw-Hill, **2003**.
- A. M. Halern and G. C. McBane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd Ed., W. H. Freeman and Company, **2006**.
- P. C. Kamboj, *University Practical Chemistry*, 1st Ed., Vishal Publishing, **2013**.
- S. K. Maity and N. K. Ghosh, *Physical Chemistry Practical*, NCBA, **2015**.
- A. K. Nad, B. Mahapatra and A. Ghoshal, *An Advanced Course in Practical Chemistry*, 3rd Ed., New Central Book Agency, **2014**.
- J. B. Yadav, *Advanced Practical Physical Chemistry*, Krishna Prakashan Media, **2010**.
- B. Viswanathan and P. S. Raghavan, *Practical Physical Chemistry*, Viva Books, **2009**..

SEMESTER – V

PAPER CODE: CHE DMT 501/CHE IDMT 503: Photochemistry, Catalysis, Quantum Chemistry & Spectroscopy

Full Mark 100 (60 + 40)

Course Objectives: The learners Able to: Understand the basic difference between thermal and photochemical processes and laws of photochemistry. Type of catalysts, specificity, selectivity, mechanism of catalyzed reaction at solid surface. Kinetics of complex reactions

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

[CHE DMT 501/CHE IDMT 503.1]. Understand the basics of photochemical processes and laws of photochemistry

[CHE DMT 501/CHE IDMT 503.2]. Learn about the basics of catalysts and classifications and chemical reactions.

[CHE DMT 501/CHE IDMT 503.3]. Learn about the kinetics of complex reactions and its mechanisms.

[CHE DMT 501/CHE IDMT 503.4]. Understand the spectroscopy and its importance in chemistry.

[CHE DMT 501/CHE IDMT 503.5]. Understand the concepts of quantum chemistry and spectroscopy.

B. SYLLABUS

Unit – I: Photochemistry

Characteristics of electromagnetic radiation and interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry: Grothus-Drapper law, Stark-Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing). Lambert-Beer's law and its limitation, physical significance of absorption coefficient; quantum efficiency, reasons for low and high quantum efficiency. Kinetics of photochemical reactions ($H_2 + Br_2 = HBr$ and $2HI = H_2 + I_2$), photostationary state. Chemical actinometers (ferri-oxalate, uranyl oxalate, MGL [malachite green leucocyanide)] and Reinecke's salt); chemiluminescence, role of photochemical reactions in biological process.

Unit – II Catalysis

Type of catalysts, specificity and selectivity, mechanism of catalyzed reaction at solid surface; effect of temperature on surface reaction, promoters and poisons.

***Heterogeneous Catalysis* (*Surface Reactions*):** Physical adsorption, chemisorptions, nature of adsorbed state, adsorption isotherm; Langmuir and Freundlich adsorption isotherms. Multi-layer adsorption-BET equation (no derivation) and its application to surface area measurement.

Kinetics Homogeneous Catalysis: Nature of surface, concept of active centres. Kinetics of enzymatic reactions: Michaelis-Menten equation, Lineweaver-Burk and Eadie plot, effect of temperature and pH.

Unit – III: Complex reactions

Kinetics of complex reactions (integrated rate expressions up to first order only): (i) opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state

approximation in reaction mechanisms) (iv) chain reactions (v) uni molecular gas reaction (Lindemann mechanism)

Unit – IV Quantum Chemistry and Spectroscopy – I

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra. Born-Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.
Postulates of quantum mechanics, quantum mechanical operators.
Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wave functions, concept of zero-point energy.

Unit – V Quantum Chemistry and Spectroscopy – II

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.
Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.
Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.
Electronic Spectroscopy: Electronic excited states. Free Electron model and its application to electronic spectra of polyenes. Color and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

Reference Books:

- P. Atkins, J. d. Paula and K. James, *Physical Chemistry*, 11th Ed., Oxford University Press, **2018**.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw-Hill, **1996**.
- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, 2nd Ed., Oxford University Press, **2007**.
- A. Chandra, *Introductory Quantum Chemistry*, 4th Ed., McGraw Hill Education, **2017**.
- T. Engel and P. Reid, *Quantum Chemistry and Spectroscopy*, 5th Ed., Pearson, **2011**.
- K. L. Kapoor, *A Text Book of Physical Chemistry: Quantum Chemistry and Molecular Spectroscopy, Vol. 4*, 5th Ed., McGraw-Hill, **2015**.
- K. J. Laidler, *Chemical Kinetics*, 3rd Ed., Pearson, **2011**.
- I. N. Levine, *Quantum Chemistry*, 7th Ed., Pearson, **2014**.
- D. A. McQuarrie and J. D. Simon, *Physical Chemistry: A Molecular Approach*, Viva Book Private Limited, **2005**.
- R. K. Prasad, *Quntum Chemistry*, 4th Ed., New Age International, **2020**.
- B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Ed., Vishal Publishing Co., **2018**.
- J. Rajaram and J. C. Kuriacose, *Kinetics and Mechanisms of Chemical Transformations*, Penguin Books Ltd, **2009**.

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
CHE DMT 501/CHE IDMT 503.1	Understand the basics of photochemical processes and laws of photochemistry	2					1	2		1		2
CHE DMT 501/CHE IDMT 503.2	Learn about the basics of catalysts and classifications and chemical reactions.	2		3			1	2	2	1		2
CHE DMT 501/CHE IDMT 503.3	Learn about the kinetics of complex reactions and its mechanisms.	2	2	2	3	1			2			1
CHE DMT 501/CHE IDMT 503.4	Understand the spectroscopy and its importance in chemistry.	1	1						2			3
CHE DMT 501/CHE IDMT 503.1.5	Understand the concepts of quantum chemistry and spectroscopy.	1		3	1			1	1			3

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

PAPER CODE: CHE DMP 507/CHE IDMP 508: Physical Chemistry Practical – III

Full Mark 50

A. SYLLABUS

Catalysis:

- Kinetics of enzymation reaction (starch-amylase system).
- Kinetics of catalytic decomposition of H_2O_2

Surface Chemistry:

- Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Photochemistry:

- Photochemical reduction of ferric oxalate in cyanotype blue printing.

UV/Visible spectroscopy:

- Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
- Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
- Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colorimetry:

- Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration.
- Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
- Study the kinetics of iodination of propanone in acidic medium.
- Determine the amount of iron present in a sample using 1,10-phenathroline.
- Determine the dissociation constant of an indicator (phenolphthalein).
- Study the kinetics of interaction of crystal violet/phenolphthalein with sodium hydroxide.
- Analysis of the given vibration-rotation spectrum of HCl(g)

Reference Books:

- J. Elias, *A Collection of Interesting General Chemistry Experiments*, Revised Ed., University Press, **2007**.
- C. W. Garland, J. W. Nibler and D. P. Shoemaker, *Experiments in Physical Chemistry*, 8th Ed., McGraw-Hill, **2003**.
- A. M. Halern and G. C. McBane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd Ed., W. H. Freeman and Company, **2006**.
- S. K. Maity and N. K. Ghosh, *Physical Chemistry Practical*, NCBA, **2015**.
- A. K. Nad, B. Mahapatra and A. Ghoshal, *An Advanced Course in Practical Chemistry*, 3rd Ed., New Central Book Agency, **2014**.
- J. B. Yadav, *Advanced Practical Physical Chemistry*, Krishna Prakashan Media, **2010**.
- B. Viswanathan and P. S. Raghavan, *Practical Physical Chemistry*, Viva Books, **2009**.

PAPER CODE: CHE DMT/I 505: Chemistry Research Orientation

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Understand the basic ideas on chemistry research and its outline. Understand the chemical safety and ethical handling of chemicals.

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

[CHE DMT/I 505.1]. Learn the ideas on research overview and importance of chemistry research.

[CHE DMT/I 505.2]. Learn about the basics of research related topics with the help of Journals, Reviews, monographs, dictionaries, text-books etc.

[CHE DMT/I 505.3]. Learn about the chemical safety and ethical handling of chemicals.

B. SYLLABUS

Unit – I: Why Students Interested on Chemistry Research?

Research Overview, Importance of Chemistry Research, Types of application in today's chemistry

Unit – II: Research Outline

Before start the research area/topic search outline of the research related topics with the help of Journals, Reviews, monographs, dictionaries, text-books etc.

Digital Sources: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider.

Outline of Journals: Elsevier, ACS, RSC, Springer, Wiley, MDPI etc.

Article format: Title, Authors, Affiliation, Abstract, Keywords, Introduction, Experimental Section, Characterization, Results & Discussion, Conclusion, Acknowledgements & References

Unit – III: Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

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
CHE DMT/I 505.1	Learn the ideas on research overview and importance of chemistry research.	2					1	2		1		2
CHE DMT/I 505.2	Learn about the basics of research related topics with the help of Journals, Reviews, monographs, dictionaries, text-books etc.	2		3			1	2	2	1		2
CHE DMT/I 505.3	Learn about the chemical safety and ethical handling of chemicals.	2	2	2	3	1			2			1

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

PAPER CODE: CHE DMP/I 509: Organic Chemistry Practical – II

Full Mark 50

Course Objectives: The learners should be able to: Learn the quantitative analysis of organic compounds.

A. SYLLABUS

Quantitative analysis

A. Organic preparations (Any six organic preparation from the following suggested topics have to be completed)

a. Acetylation of one of the following compounds: amines (aniline, o-, m-, p-toluidines and o-, m-, p-anisidine) and phenols (β-naphthol, vanillin, salicylic acid) by any one method:
   1. Using conventional method
   2. Using Green Method

b. Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and one of the following phenols (β-naphthol, resorcinol, p-cresol) by Schotten-Baumann reaction.

c. Oxidation of ethanol/ isopropanol (Iodoform reaction).

d. Bromination of any one of the following:
   1. Acetanilide by conventional methods
   2. Acetanilide using green approach (Bromate-bromide method)

e. Nitration of any one of the following:
   1. Acetanilide/nitrobenzene by conventional method
   2. Salicylic acid by green approach (using ceric ammonium nitrate)

f. Reduction of p-nitrobenzaldehyde by sodium borohydride.

g. Hydrolysis of amides and esters.

h. Aldol condensation: Preparation of chalcone substrate.

i. Azo compound preparation (Methyl orange)

j. Racemic BINOL preparation from β-naphthol using $FeCl_3$.

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and TLC.

B. Estimation (Any Three estimations from the following experiments have to be done)

a. Estimation of glycine by Sorenson's formalin method.
b. Study of the titration curve of glycine.
c. Saponification value of an oil or a fat.
d. Determination of Iodine number of an oil/ fat.
e. Isolation and characterization of DNA from onion/ cauliflower/peas.

Reference Books:

- Mann, F.G. & Saunders, B.C. Practical Organic Chemistry, Pearson Education (2009)
- Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G.; Tatchell, A.R. Practical Organic Chemistry, 5th Ed., Pearson (2012)
- Ahluwalia, V.K. & Aggarwal, R. Comprehensive Practical Organic Chemistry: Preparation and Quantitative Analysis, University Press (2000).
- Ahluwalia, V.K. & Dhingra, S. Comprehensive Practical Organic Chemistry, Qualitative Analysis, University Press (2002). Manual of Biochemistry Workshop, 2012, Department of Chemistry, University of Delhi.
- Arthur, I. V. Quantitative Organic Analysis, Pearson.

SEMESTER – VI

PAPER CODE: CHE DMT 601/CHE IDMT 604: Coordination & Organometallics Chemistry

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basics coordination compounds and its properties and applications. Understand the concepts of electronic spectra and magnetic properties of transition metal complexes, bioinorganic chemistry and organometallics chemistry.

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

[CHE DMT 601/CHE IDMT 604.1]. Understand the isomerism, properties and applications of coordination compounds.

[CHE DMT 601/CHE IDMT 604.2]. Introductory of electronic spectra of transition metal complexes and applications.

[CHE DMT 601/CHE IDMT 604.3]. Learn the magnetic properties and applications of transition metals.

[CHE DMT 601/CHE IDMT 604.4]. Understand the importance bioinorganic chemistry in daily life.

[CHE DMT 601/CHE IDMT 604.5]. Understand the organometallics compounds structure, bonding properties and applications.

B. SYLLABUS

Unit – I: Coordination Chemistry

Werner's theory, IUPAC nomenclature of coordination compounds, Types of isomerism in coordination compounds: Constitutional, geometrical and optical isomerism in respect of coordination numbers 4 and 6, Determination of configuration of cis-, trans-isomers by chemical methods.

Valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (o, t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory, Chelate effect, polynuclear complexes.

Unit – I: Electronic Spectra of Transition Metal Complex

Introduction to electronic spectra of transition metal complexes, Orgel diagrams for $3d^1$-$3d^9$ ions, selection rules, d-d/charge transfer spectra, Colour, spectrochemical series, Nephelauxetic effect, trans effect, (example and applications) labile and inert complexes. Difference between the first, second and third transition series.

Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy)

Unit – III: Magnetic Properties of Transition Metal

Types of magnetic behaviour, methods of determining magnetic susceptibility, spin only formula, L-S coupling, Orbital contribution to magnetic moments, quenching of magnetic moment, super-exchange, antiferromagnetic interaction (elementary idea with examples only), application of spin only values of magnetic moments to determine valency and stereochemistry of coordination compounds (based on VBT and CFT)

Unit – IV: Bioinorganic Chemistry

Elements of life: essential major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na^{+}, K^{+}, Mg^{+2}, Ca^{+2}, $Fe^{3+/2+}$, Cu^{+2}, and Zn^{+2}). Haemoglobin, myoglobin, chlorophyll, cytochromes, ferredoxins and carbonic anhydrase-their structural features and functions in living system.

Toxic metal ions and their effects, lead, mercury, cadmium and arsenic poisoning, organo-mercury compounds; Use of chelating agents in medicine: Wilson diseases, detoxification of metal ions – chelation therapy (simple idea with some examples of chelating drugs). Pt and Au complexes as drugs (examples only), metal dependent diseases.

Unit – V: Organometallic Chemistry

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands.

Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition), Structures of mono and binuclear carbonyls of 3d series.

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls, Metal Alkyls: Important structural features of different allyl compounds. Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Catalysts: Study of the following industrial processes and their reactions & mechanism: Alkene hydrogenation (Wilkinsons Catalyst), Hydroformylation (Co salts), Wacker Process, Synthetic gasoline (Fischer Tropsch reaction), Synthesis gas by metal carbonyl complexes.

Reference Books:

- Purcell, K.F & Kotz, J.C. Inorganic Chemistry W.B. Saunders Co, 1977.
- Huheey, J.E., Inorganic Chemistry, Prentice Hall, 1993.
- Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry Panima Publishing Company 1994.
- Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH, 1999
- Basolo, F, and Pearson, R.C., Mechanisms of Inorganic Chemistry, John Wiley & Sons, NY, 1967.

Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, Butterworth-Heinemann, 1997.

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
CHE DMT 601/CHE IDMT 604.1	Understand the isomerism, properties and applications of coordination compounds.	2					1	2		1		2
CHE DMT 601/CHE IDMT 604.2	Introductory of electronic spectra of transition metal complexes and applications.	2		3			1	2	2	1		2
CHE DMT 601/CHE IDMT 604.3	Learn the magnetic properties and applications of transition metals.	2	2	2	3	1			2			1
CHE DMT 601/CHE IDMT 604.4	Understand the importance bioinorganic chemistry in daily life.	1	1						2			3
CHE DMT 601/CHE IDMT 604.5	Understand the organometallics compounds structure, bonding properties and applications.	1		3	1			1	1			3

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

PAPER CODE: CHE DMP 607/CHE IDMP 608: Inorganic Chemistry Practical – III

Full Mark 50

Course Objectives: The learners should be able to: Learn the quantitative analysis of inorganic salts.

A. SYLLABUS

(A) Qualitative Estimation of unknown salts

Qualitative semimicro analysis of mixtures containing 2 anions and 2 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, CH_3COO^-, F^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}

Mixtures should preferably contain one interfering anion, **or** insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) **or** combination of anions e.g. $CO_3^{2-}$and SO_3^{2-}, NO_2^- and NO_3^-, Cl^- and Br^-, Cl^- and I^-, Br^- and I^-, NO_3^- and Br^-, NO_3^- and I^-.

Spot tests should be done whenever possible

i. Measurement of 10 Dq by spectrophotometric method
ii. Verification of spectrochemical series.
iii. Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.
iv. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

(B) Iodo / Iodimetric Titrations

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).
(ii) Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically
(iii) Estimation of available chlorine in bleaching powder iodometrically.

Reference Books

- Vogel's *Qualitative Inorganic Analysis,* Revised by G. Svehla.
- Marr & Rockett *Inorganic Preparations.*
- Ghosal, Mahapatra and Nad, *An Advanced Course in Practical Chemistry*.

PAPER CODE: CHE DMT 603/CHE DMT 608: Bioorganic Chemistry

Full Mark 100 (60 + 40)

Course Objectives: The learners are Able to: Learn the basics of classifications, importance, structure, properties and chemical reactions of carbohydrates, Amino acids, Peptides, Proteins, Lipids, Nucleic Acids and Natural Products.

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

[CHE DMT 603/CHE DMT 608.1]. Learn the classifications, importance, structure, properties and chemical reactions of carbohydrates

[CHE DMT 603/CHE DMT 608.2]. Learn the classification, importance, properties and chemical reactions of Amino acids, Peptides, Proteins.

[CHE DMT 603/CHE DMT 608.3]. Understand the classifications and properties and chemical reactions of Lipids, Nucleic Acids.

[CHE DMT 603/CHE DMT 608.4]. Understand the basics properties and chemical reactions of N-containing Functional Groups and Heterocyclic compounds.

[CHE DMT 603/CHE DMT 608.5]. Understand the basics classifications and properties and chemical reactions of Natural Products.

B. SYLLABUS

Unit – I: Carbohydrates

Classification, Monosaccharides, erythro-andthreo-(D/L) sugars, epimers, cyclicstructures of monosaccharides, Haworth projections and other conformational structures, Interconversion of aldoses and ketoses, mutarotation, chain-shortening and lengthening of sugars (Killiani-Fischer synthesis and Ruff degradation), reactions of monosaccharides, reducing and nonreducing sugars, proof of configuration, determinationof ring size, disaccharides (Only structure and properties: maltose, lactose and sucrose) and polysaccharides (Starch, cellulose and glycogen).

Unit – II: Amino acids, Peptides and Proteins

Classification and nomenclature of amino acids, configuration, acid-base properties, isoelectric point, Amino acid synthesis and chemical properties of amino acids. Peptides: peptide bond, sequencing a peptide (N-terminus and C-terminus), Peptide synthesis: solution and solid phase peptide synthesis, biologically importantpeptides (glutathione, oxytocin-important functions). Proteins: Structure of proteins (Primary, Secondary,Tertiary, Quaternary- definition, examples). Forces that stabilize structure of proteins: H-bonds,hydrophobic interaction, electrostatic attraction, Van der Waal's interaction, dipole-dipoleinteraction.

Unit – III: Lipids and Nucleic Acids

Introduction to lipids, Waxes, Triglycerides, Reaction of triglycerides, Phospholipids, Steroids (Cholesterol), Prostaglandin: Structure and functions

Nucleic Acids: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding, structure of ribonucleic acid (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical synthesis of mono and tri nucleosides. Chemical Properties: Hydrolysis (acid, alkali), enzymatic hydrolysis of DNA. General structure and types of RNA (tRNA,

mRNA, rRNA).

Unit – IV: N-containing Functional Groups and Heterocyclic Chemistry N-containing Functional Groups

Introduction to amines, Nomenclature and classification of amines, Properties of amines, Strategies of amine synthesis (via substitution reactions, Reductive amination and Gabriel Phthalimide synthesis), acylation and sulfonylation of amines, Reactions of amines with nitrous acids, Aryl Diazonium salt preparations and reactions (Sandmeyer Reaction).

Heterocyclic Chemistry

Introduction to heterocyclic chemistry, Basics of structures, nomenclature, properties, Synthesis and properties of Furan, Thiophene and Pyrrole, Indole.

Unit – V: Natural Products

Basics of Terpenoids and alkaloids, Isolation and structure elucidation of Terpenoids (Citral, Geraniol, Menthol), alkaloids (Nicotine, atropine).

C. Reference Books:

1. Modern Methods of Organic Synthesis-By Willium Carruthers and Ian Coldham
2. Organic Chemistry (2nd Edition)-By Jonathan Clayden, Nick Greeves and Stuart warren
3. Organic Chemistry (3rd Edition)-By David Klein
4. Organic Chemistry (8th Edition)-By Paula YurkanisBruice

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 603/CHE DMT 608.1	Learn the classifications, importance, structure, properties and chemical reactions of carbohydrates	2					1	2		1		2
CHE DMT 603/CHE DMT 608.2	Learn the classification, importance, properties and chemical reactions of Amino acids, Peptides, Proteins.	2		3			1	2	2	1		2
CHE DMT 603/CHE DMT 608.3	Understand the classifications and properties and chemical reactions of Lipids, Nucleic Acids.	2	2	2	3	1			2			1
CHE DMT 603/CHE DMT 608.4	Understand the basics properties and chemical reactions of N-containing Functional Groups and Heterocyclic compounds.	1	1						2			3
CHE DMT 603/CHE DMT 608.5	Understand the basics classifications and properties and chemical reactions of Natural Products.	1		3	1			1	1			3

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

SEMESTER – VII

(Honours / PG Course)

PAPER CODE: CHE DMT 701: 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

[CHE DMT 701.1]. Understand the Co-ordination chemistry of transition metal compounds.
[CHE DMT 701.2]. Learn about the electronic spectra of transition metal complexes and their studies.
[CHE DMT 701.3]. Learn about the magnetic properties of transition series metals, lanthanides and actinides.
[CHE DMT 701.4]. Apply concepts on Inorganic reaction mechanism and electron transfer reactions.
[CHE DMT 701.5]. 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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 701.1	Understand the Co-ordination chemistry of transition metal compounds	2					1	2		1		2
CHE DMT 701.2	Learn about the electronic spectra of transition metal complexes and their studies.	2		3			1	2	2	1		2
CHE DMT 701.3	Learn about the magnetic properties of transition series metals, lanthanides and actinides.	2	2	2	3	1			2			1
CHE DMT 701.4	Apply concepts on Inorganic reaction mechanism and electron transfer reactions.	1	1						2			3
CHE DMT 701.5	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: CHE DMP 705: Inorganic Practical – III

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).

SYLLABUS

(A) Gravimetric Analysis:

i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
ii. Estimation of copper as CuSCN
iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.
iv. Estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

(B) Inorganic Preparations:

i. Tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
ii. *Cis* and *trans* $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)
iii. Tetraamminecarbonatocobalt (III) ion
iv. Potassium tris(oxalate)ferrate(III)

(C) Chromatography Separation of metal ions

- Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

i. Ni (II) and Co (II)
ii. Fe (III) and Al (III)

- Chromatographic separation of sugars, amino acids by paper, T.L.C. and Ion exchange.

(D) Estimation of $Fe^{2+/3+}$, Cu^{2+}, Ca^{2+} ions from dichromate/thiosulphate solution.

Reference Book:

1. Vogel, A.I. A text book of Quantitative Analysis, ELBS 1986.

PAPER CODE: CHE DMT 702: 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

[CHE DMT 702.1]. Understand the physical properties (thermodynamic and kinetic) of organic reactions. **[CHE DMT 702.2].** Learn about substitution, addition, and elimination of organic reactions.
[CHE DMT 702.3]. Understand the symmetry properties, stereoisomerism and stereospecific reactions.
[CHE DMT 702.4]. Learn the principle and concepts of organic compounds chirality and conformations.
[CHE DMT 702.5]. 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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 702.1	Understand the physical properties (thermodynamic and kinetic) of organic reactions.	2					1	2		1		2
CHE DMT 702.2	Learn about substitution, addition, and elimination of organic reactions.	2		3			1	2	2	1		2
CHE DMT 702.3	Understand the symmetry properties, stereoisomerism and stereospecific reactions.	2	2	2	3	1			2			1
CHE DMT 702.4	Learn the principle and concepts of organic compounds chirality and conformations.	1	1						2			3
CHE DMT 702.5	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: CHE DMP 706: 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*.

PAPER CODE: CHE DMT 703: 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

[CHE DMT 703.1]. Recall basic concepts of thermodynamics, excess function for non-ideal solutions.
[CHE DMT 703.2]. Understand the heterogeneous catalysis via surface reactions.
[CHE DMT 703.3]. Understand the Kinetics of homogeneous catalysis.
[CHE DMT 703.4]. Discuss the electrical double layer and metal/electrolyte interface.
[CHE DMT 703.5]. Discuss the basics concepts of surface tension and surface active agents.

B. 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.

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**.

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

COURSE	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 703..1	Recall basic concepts of thermodynamics, excess function for non-ideal solutions.	3		2				2	2			2
CHE DMT 703..2	Understand the heterogeneous catalysis via surface reactions.	2	2				2		2	1		1
CHE DMT 703..3	Understand the Kinetics of homogeneous catalysis.	1			2		2				3	2
CHE DMT 703..4	Discuss the electrical double layer and metal/electrolyte interface.	2		1			2			2	2	2
CHE DMT 703..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: CHE DMT (I) 704: Research Methodology for Chemistry

Full Mark 50 (30 + 20)

Unit – I: Literature Survey

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups andcommunities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry for finding and citing published information from Science Direct, SciFinder, Scopus.

Unit – II: Methods of Scientific Research and Writing Scientific Papers

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

Unit –III: Research Ethics and Data Analysis

Research Ethics: Copy-writing, Scientific Interpretation, Data manipulation etc. strictly offensive and it should avoid.

Data Analysis

The Investigative Approach: Making and Recording Measurements of experimental products by using sophisticated instruments. Analysis raw data interpret by using different software like Chem-draw, Origin, Excels etc.

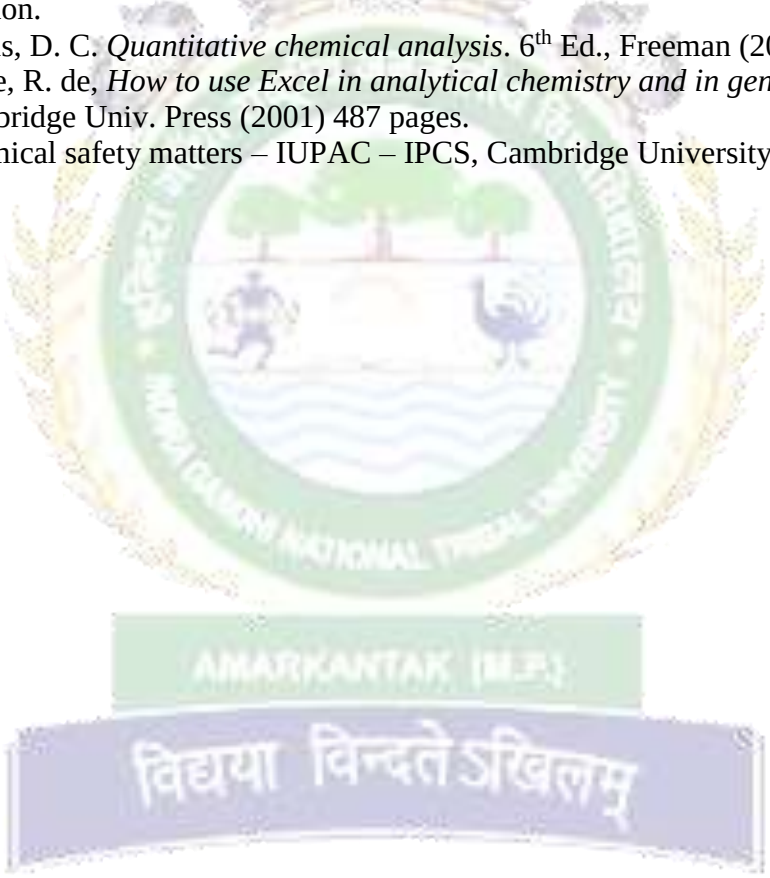
Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial

fitting, linearizing transformations, exponential function fit, *r* and its abuse. Basic aspects of multiple linear regression analysis.

Electronics: Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

Reference Books

- Dean, J. R., Jones, A. M., Holmes, D., Reed, R., Weyers, J. & Jones, A. (2011) *Practical skills in chemistry*. 2nd Ed. Prentice-Hall, Harlow.
- Hibbert, D. B. & Gooding, J. J. (2006) *Data analysis for chemistry*. Oxford University Press.
- Topping, J. (1984) *Errors of observation and their treatment.* Fourth Ed., Chapman Hall, London.
- Harris, D. C. *Quantitative chemical analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis.* Cambridge Univ. Press (2001) 487 pages.
- Chemical safety matters – IUPAC – IPCS, Cambridge University Press, 1992.



PAPER CODE: CHE DMP/I 707: Chemistry Software Uses for Advanced Research

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(Full Mark 50 (30 + 20)

1. Practical Assignment: Graph plot of XRD, FTIR, UV by apply Origine software,
2. Chemical Structure Draw by using Chem Draw software
3. Seminar
4. Short Project Work

SEMESTER – VIII

(PG Course)

(Credits: 20; Laboratory & Other Activities: 6 Months; Maximum Marks: 500)

PAPER CODE: CHE D 801: Project & 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. The project work is evaluated by the fulfilment of the following criteria.

	Course Code	Criteria	Credit	Marks
Dissertation/ Project	**CHE D 801**	**D 801: Dissertation/Project**		
	CHE D 801A	• D 801A: Development of project/ Research proposal/Lab Work	**4**	**100**
	CHE D 801B	• D 801B: Pre-Submission presentation/Data collection	**4**	**100**
	CHE D 801C	• D 801C: Report Writing/Write-up/ Dissertation Report	**8**	**200**
	CHE D 801D	• D 801D: Presentation &Viva Voce	**4**	**100**
		Total	**20**	**500**

SEMESTER – IX

(PG Course)

PAPER CODE: CHE DMT 901: Organometallic Chemistry

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

[CHE DMT 901.1]. Understand the basic concepts of organo transition metal chemistry.

[CHE DMT 901.2]. Learn about the chemical reactions, mechanism, and catalysis of organometallic complexes.

[CHE DMT 901.3]. Learn about the structure and bonding of inorganic rings, cages and clusters.

[CHE DMT 901.4]. Provide insights into structure, property and applications of organometallic complexes.

[CHE DMT 901.5]. 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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 901.1	Understand the basic concepts of organo transition metal chemistry.	2					1	2		1		2
CHE DMT 901.2	Learn about the chemical reactions, mechanism, and catalysis of organometallic complexes.	2		3			1	2	2	1		2
CHE DMT 901.3	Learn about the structure and bonding of inorganic rings, cages and clusters.	2	2	2	3	1			2			1
CHE DMT 901.4	Provide insights into structure, property and applications of organometallic complexes.	1	1						2			3
CHE DMT 901.5	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: CHE DMP 905: Inorganic Chemistry Practical – IV

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. Qualitative Analysis

Semi-micro qualitative analysis of mixture containing six 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. Mixture Separation of Inorganic metal ions:

- 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 by gravimetrically /complexometrically/spectrophotometrically.

C. Preparations of Complex

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, Mercury tetrathiocyanatocobaltate(II), Copper(II) biguanide
4. Mn_{12} Acetate Single Molecule Magnet
5. Preparation of copper glycine complex- cis and transbis- (glycinato) copper (II).
6. 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).
7. VO(*acac*)$_2$, *cis*-K $[Cr(C_2O_4)_2(H_2O)_2]$, $Na[Cr(NH_3)_2(SCN)_4]$

Reference Books:

- A.I. Vogel: *Qualitative Inorganic Analysis*, Prentice Hall, 7th Edn.
- A.I. Vogel: *Quantitative Chemical Analysis*, Prentice Hall, 6th Edn.
- B.D. Khosla: *Senior Practical Physical Chemistry*, R. Chand & Co.
- P. C. Comboj: *University Practical Chemistry*, Vishal Publishing Co. Jalandhar.
- *Vogel's Textbook of Quantitative Analysis*, Revi Mendham, ELBS.

- W.L. Jolly, *Synthesis and Characterization of Inorganic Compounds*, Prentice Hall.

PAPER CODE: CHE DMT 902: Principle of Organic Synthesis

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

[CHE DMT 902.1]. Understand the basic principles of organic synthesis and acid base catalyzed reactions. **[CHE DMT 902.2].** Learn about rearrangement and organometallic and organic reactions. **[CHE DMT 902.3].** Understand the symmetry properties, stereoisomerism and stereospecific reactions. **[CHE DMT 902.4].** Learn the Understand the UV, IR, and NMR spectroscopy analysis of organic compounds.
[CHE DMT 902.5]. 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.

(12 Hours)

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.

(12 Hours)

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.

(14 Hours)

Unit – 5: Structure Determination of Organic Compounds

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

(10 Hours)

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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 902.1	Understand the basic principles of organic synthesis and acid base catalyzed reactions.	2					1	2		1		2
CHE DMT 902.2	Learn about rearrangement and organometallic and organic reactions.	2		3			1	2	2	1		2
CHE DMT 902.3	Understand the symmetry properties, stereoisomerism and stereospecific reactions.	2	2	2	3	1			2			1
CHE DMT 902.4	Learn the Understand the UV, IR, and NMR spectroscopy analysis of organic compounds.	1	1						2			3
CHE DMT 902.5	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: CHE DMP 906: Organic Chemistry Practical – IV

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.

- Nitrobenzene→aniline→Acetanilide (Nitration and followed by reduction)
- Malonic acid→cinnamicacid→methylcinnamate (Knoevenagel 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→cinnamylalcohol→cinnamylbromide→allyl-aryl ether synthesis (Nucleophilic substitution reaction)

Part B: Characterization of above said synthesized organic compounds using IR, UV and NMR, and mass spectroscopic techniques are to be studied.
Part C: Designing and drawing a reaction scheme and structures using Chemdraw software.

Reference Books:

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

PAPER CODE: CHE DMT 903: Quantum-, Statistical- Mechanics, Chemical Kinetics

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

[CHE DMT 903.1]. Learn about the historic background of quantum mechanics versus classical mechanics.
[CHE DMT 903.2]. Understand the Schrödinger wave equation in spherical coordinates, rigid rotor.
[CHE DMT 903.3]. Understand the basic principles of atomic structure, term symbols and spectroscopic states.
[CHE DMT 903.4]. Able to learn the principles and techniques of statistical thermodynamics.
[CHE DMT 903.5]. Apply the concepts of chemical kinetics of reactions in gas and solution phase.

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: Chemical Kinetics

Rate law, method of determining rate laws, General feature of fast reactions, study of fast reaction by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

Reactions in Gas Phase: Theories of Reaction Rates- Arrhenius theory, collision theory and transition state theory, potential energy surface, enthalpy, free energy and entropy of activation, correlation of steric factor in collision theory and entropy of activation (Thermodynamic parameter). Uni-molecular reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kasssel (RRK) theory, Rice- Ramsperger-Kassel-Marcus (RRKM) theory.

***Elementary Reactions in Solution*:** Comparison between gas-phase and solution-phase reactions, factor determining reaction rates in solution; ionic reaction [influence of solvent, influence of ionic strength (salt effect)] ; Linear Free Energy Relationships, (LFER), Effect of substituent on reaction rates (Hammet relationships). Kinetic of isotopic effects.

***Dynamic of Molecular Motion*:** probing the transition state, dynamics of barrier-less chemical reaction in solution.

Chain Dynamic: (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reaction), and Oscillatory reaction, autocatalysis (Belousov-Zhabotinsky reaction).

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	PC 3	PC 4	PC 5	PC 6	PO 7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 903.1	Learn about the historic background of quantum mechanics versus classical mechanics.	3		2				2	2			2
CHE DMT 903.2	Understand the Schrödinger wave equation in spherical coordinates, rigid rotor.	2	2				2		2	1		1
CHE DMT 903.3	Understand the basic principles of atomic structure, term symbols and spectroscopic states.	1			2		2				3	2
CHE DMT 903.4	Able to learn the principles and techniques of statistical thermodynamics.	2		1			2			2	2	2
CHE DMT 903.5	Apply the concepts of chemical kinetics of reactions in gas and solution phase.	2		1		3		2	2			3

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

PAPER CODE: CHE DET 904: 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

[CHE DET 904.1]. Understand the basic principles and interaction of electromagnetic radiation with matter.

[CHE DET 904.2]. Apply the concepts of microwave (rotational) spectroscopy techniques.

[CHE DET 904.3]. Learn the basic principles and applications of vibrational (IR and Raman) spectroscopy.

[CHE DET 904.4]. Learn the concepts of electronic (atomic, molecular, and photoelectron) spectroscopies.

[CHE DET 904.5]. 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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DET 904.1	Understand the basic principles and interaction of electromagnetic radiation with matter.	2					1	2		1		2
CHE DET 904.2	Apply the concepts of microwave (rotational) spectroscopy techniques.	2		3			1	2	2	1		2
CHE DET 904.3	Learn the basic principles and applications of vibrational (IR and Raman) spectroscopy.	2	2	2	3	1			2			1
CHE DET 904.4	Learn the concepts of electronic (atomic, molecular, and photoelectron) spectroscopies.	1	1						2			3
CHE DET 904.5	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

SEMESTER – X (PG Course)

PAPER CODE: CHE DMT 1001: Bio-Inorganic & Sensor Materials 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

[CHE DMT 1001.1]. Learn the basic structure, bonding advanced bio-inorganic chemistry in daily life.

[CHE DMT 1001.2]. Learn about basic properties of metallic enzymes, carbonic anhydrase and etc.

[CHE DMT 1001.3]. Learn about the magnetic properties of transition series metals, lanthanides and actinides.

[CHE DMT 10014]. Understand the basic concepts introduction of inorganic photochemistry, photophysical and photochemical process.

[CHE DMT 1001.5]. Learn the concept of molecular recognition and metal ion sensing nanomaterials.

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: Sensor Materials Chemistry

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.

Different types of Sensing Materials

Metal ion sensing nanomaterials, Dyes sensing nanomaterials, MOFs used as sensing materials, Nanomaterials are used in therapeutic treatment

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.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 1001.1	Learn the basic structure, bonding advanced bio-inorganic chemistry in daily life.	2					1	2		1		2
CHE DMT 1001.2	Learn about basic properties of metallic enzymes, carbonic anhydrase and etc.	2		3			1	2	2	1		2
CHE DMT 10013	Learn about the magnetic properties of transition series metals, lanthanides and actinides.	2	2	2	3	1			2			1
CHE DMT 1001.4	Understand the basic concepts introduction of inorganic photochemistry, photophysical and photochemical process.	1	1						2			3
CHE DMT 1001.5	Learn the concept of molecular recognition and metal ion sensing nanomaterials	1		3	1			1	1			3

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

PAPER CODE: CHE DMT 1002: 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

[CHE DMT 1002.1]. Understand the basic introduction of pericyclic reactions.

[CHE DMT 1002.2]. Learn about the electrocyclic and cycloaddition reactions of pericyclic compounds.

[CHE DMT 1002.3]. Learn about the classification of sigmatropic rearrangement reaction and mechanism. **[CHE DMT 1002.4].** Apply concepts on photochemistry and reaction with carbonyl compounds.

[CHE DMT 1002.5]. 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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 1002.1	Understand the basic introduction of pericyclic reactions	2					1	2		1		2
CHE DMT 1002.2	Learn about the electrocyclic and cycloaddition reactions of pericyclic compounds.	2		3			1	2	2	1		2
CHE DMT 1002.3	Learn about the classification of sigmatropic rearrangement reaction and mechanism.	2	2	2	3	1			2			1
CHE DMT 1002.4	Apply concepts on photochemistry and reaction with carbonyl compounds.	1	1						2			3
CHE DMT 1002.5	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: CHE DMT 1003: Chemical Bonding, Group Theory, and Solid State Chemistry

Full Mark 100 (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 symmetry & group theory and applications and solid state chemistry, crystals defects and magnetic properties.

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

[CHE DMT 1003.1]. Understand the chemical bonding in diatomic molecules and elementary concepts of MO and VB theories.

[CHE DMT 1003.2]. Introductory of semi-empirical and *ab-initio* calculations on molecular systems.

[CHE DMT 1003.3]. Apply concepts on symmetry & group theory and character of a representation.

[CHE DMT 1003.4]. Learn the application of group theory to atomic orbitals and selection rules for IR and Raman spectra.

[CHE DMT 1003.5]. 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: 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.

Unit – 4: Application of Group Theory

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, SF_6, etc.

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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMT 1003.1	Understand the chemical bonding in diatomic molecules and elementary concepts of MO and VB theories.	2					1	2		1		2
CHE DMT 1003.2	Introductory of semi-empirical and *ab-initio* calculations on molecular systems.	2		3			1	2	2	1		2
CHE DMT 1003.3	Apply concepts on symmetry & group theory and character of a representation.	2	2	2	3	1			2			1
CHE DMT 1003.4	Learn the application of group theory to atomic orbitals and selection rules for IR and Raman spectra	1	1						2			3
CHE DMT 1003.5	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

PAPER CODE: CHE DET 1004A: Introduction to Nanomaterials & Nanotechnology

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

[CHE DET 1004A. 1]. Understand the background principle nanotechnology and types of nanomaterials.

[CHE DET 1004A.2]. Learn characterization techniques for the structure and properties of nanomaterials.

[CHE DET 1004A.3]. Learn the background and importance behind the synthesis of nanomaterials.

[CHE DET 1004A.4]. Understand the concepts of size dependent properties while preparing nanomaterials.

[CHE DET 1004A.5]. Understand the nanomaterial applications towards the world requirements.

A. 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); thermal techniques (TG, DTA, DSC), an introduction and basic principles & applications of XPS, FTIR spectrophotometers; UV-VIS principle and application for band gap measurement, magnetic technique-VSM/SQUID.

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.

B. 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

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DET 1004A.1	Understand the background principle nanotechnology and types of nanomaterials.	2					1	2		1		2
CHE DET 1004A.2	Learn characterization techniques for the structure and properties of nanomaterials.	2		3			1	2	2	1		2
CHE DET 1004A.3	Learn the background and importance behind the synthesis of nanomaterials.	2	2	2	3	1			2			1
CHE DET 1004A.4	Understand the concepts of size dependent properties while preparing nanomaterials.	1	1						2			3
CHE DET 1004A.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: CHE DET 1004B: Advanced Heterocyclic Chemistry

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

[CHE DET 1004B.1]. Understand the basics of aromatic and non-aromatic heterocyclic compounds.
[CHE DET 1004B.2]. Learn about the strains, interactions and conformational aspects of non-aromatic heterocycles.
[CHE DET 1004B.3]. Learn the basics on five and six membered heterocyclics with one hetero atom.
[CHE DET 1004B.4]. Learn the basic idea on synthesis and reactions of five and six membered heterocyclics with one hetero atoms.
[CHE DET 1004B.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			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DET 1004B.1	Understand the basics of aromatic and non-aromatic heterocyclic compounds.	2					1	2		1		2
CHE DET 1004B.2	Learn about the strains, interactions and conformational aspects of non-aromatic heterocycles.	2		3			1	2	2	1		2
CHE DET 1004B.3	Learn the basics on five and six membered heterocyclics with one hetero atom.	2	2	2	3	1			2			1
CHE DET 1004B.4	Learn the basic idea on synthesis and reactions of five and six membered heterocyclics with one hetero atoms.	1	1						2			3
CHE DET 1004B.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


AMARKANTAK (M.P.)
विद्यया विन्दतेऽखिलम्

PAPER CODE: CHE DMP 1005: Physical Chemistry Practical – IV

Full Mark 50

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

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.

(ii) 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.

(iii) (a) Rate of the hydrolysis of sucrose using polarimeter.

(b) Polarizability from refractive index measurement.

(iv) 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.

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

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

Reference Books:

- J. Elias, *A Collection of Interesting General Chemistry Experiments*, Revised Ed., University Press, **2007**.
- C. W. Garland, J. W. Nibler and D. P. Shoemaker, *Experiments in Physical Chemistry*, 8th Ed., McGraw-Hill, **2003**.
- A. M. Halern and G. C. McBane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd Ed., W. H. Freeman and Company, **2006**.

- S. K. Maity and N. K. Ghosh, *Physical Chemistry Practical*, NCBA, **2015**.
- A. K. Nad, B. Mahapatra and A. Ghoshal, *An Advanced Course in Practical Chemistry*, 3rd Ed., New Central Book Agency, **2014**.
- J. B. Yadav, *Advanced Practical Physical Chemistry*, Krishna Prakashan Media, **2010**.
- B. Viswanathan and P. S. Raghavan, *Practical Physical Chemistry*, Viva Books, **2009**.
- J. Rose, *Advanced Physico-Chemical Experiments: A textbook of Practical Physical Chemistry and Calculations*, Sir Isaac Pitman & Sons, **1964**.
- F. Daniels, R. A. Alberty, J. W. Williams, C. D. Cornwell, P. Bender and J. E. Harriman, *Experimental Physical Chemistry*, 7th Ed., McGraw-Hill, **1970**.

CHE DMP 1006A: Nanomaterials Chemistry Practical

Full Mark 50

Course Objectives: The learners are Able to: Learn about the basics and applications Nanomaterials.

B. SYLLABUS

Nano Materials Chemistry

- Verification of the Beer-Lambert law using gold/silver nanoparticles.
- Preparation and characterization of nanomaretials by wet chemical routes (sol-gel, reverse micelles, hydrothermal, co-precipitation, *etc*.)
- Synthesis and characterization of core-shell nanocomposite (bimetallic and oxides)
- Synthesis and characterization of mixed metal oxide (bimetallic and oxides)
- Metal based nanoparticles are examined by converting *p*-nitrophenol to *p*-aminophenol.
- Determination of the band gap of semiconductor nanomaterials.
- Study of surface enhanced Raman scattering activity of silver nanostructures.
- Study dye degradation of synthesized nanoparticles by UV/Visible light.

References:

- Furniss, B.S.; Hannaford, A.J.; Rogers, V.; Smith, P.W.G.; Tatchell, A.R. *Vogel's Textbook of Practical Organic Chemistry*, ELBS.
- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).

CHE DMP 1006B: Advanced Heterocyclic Chemistry Practical

Full Mark 50

Course Objectives: The learners are Able to: Learn about the basic studies and application of heterocyclic compounds.

A. SYLLABUS

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.

Minor Paper in Chemistry
(Disciplinary Minor/Inter-disciplinary Minor)

Minor Paper in Chemistry							
Semester	Course Code	Course Name	Marks		Total Marks	Duration (Hrs) of Exam (End Term	Credit
			END TERM	MID TERM			
I	CHE DMI 102 & CHE IDMI 104	States of Matter and Colloidal State	30	20	50	2	2
II	CHE DMI 202 & CHE IDMI 204	Chemistry in Daily Life	30	20	50	2	2
III	CHE DMI 302 & CHE IDMI 304	Basic Analytical Chemistry	30	20	50	2	2
IV	CHE DMI 402 & CHE IDMI 404	Chemical and Phase Equilibria, Solutions and Colligative Properties	30	20	50	2	2
V	CHE DMI 502 & CHE IDMI 504	Advanced Analytical Chemistry	30	20	50	2	2
VI	CHE DMI 602 & CHE IDMI 605	Organic Spectroscopy	30	20	50	2	2

The I-VI Minor disciplinary/multidisciplinary paper may be substituted by the following additional Minor papers subject to the availability of the Teacher and class load of the discipline/teacher in any semester.

Additional Course:

CHE DMI 102/ CHE IDMI 104: IT Skill for Chemist

CHE DMI 202/ CHE IDMI 204: Green Methods in Chemistry

CHE DMI 302/ CHE IDMI 304: Basic of Nanomaterials

CHE DMI 402/ CHE IDMI 404: Crystalline Materials and Properties

CHE DMI 502/ CHE IDMI 504: Inorganic Materials of Industrial Importance

CHE DMI 602/ CHE IDMI 605: Basic of Drug Design & Medicinal Chemistry

Disciplinary Minor /Inter-disciplinary Minor

SEMESTER – I

CHE DMI 102/ CHE IDMI 104: States of Matter and Colloidal State

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation, Nature of the solid state materials, physical and chemical properties of Liquid and Colloidal States.

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

[CHE DMI 102/CHE IDMI 104.1]. Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation

[CHE DMI 102/CHE IDMI 104.2]. Understand the nature of the solid state, definition of space lattice, unit cell; laws of crystallography.

[CHE DMI 102/CHE IDMI 104.3]. Learn about the classification, preparation, and properties, general application of colloids and liquids.

B. SYLLABUS

Unit – I: Gaseous State

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation.

Behavior of real gases: Deviations from ideal gas behavior, compressibility factor and its variation with pressure for different gases. Causes of deviation from ideal behavior; van der Waals equation of state, its derivation and application in explaining real gas behavior, mention of other equations of state (Berthelot, Dietrici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Maxwell Boltzmann distribution laws of molecular velocity and molecular energies (graphic representation – derivation not required) and its use in evaluating molecular velocities (average, root mean square, and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Collision frequency, collision diameter, and mean free path including their temperature and pressure dependence; viscosity of gases, relation between mean free path and coefficient of viscosity; calculation of collision diameter from coefficient of viscosity; variation of viscosity of gases with temperature and pressure.

Unit – II: Solid State

Nature of the solid state, definition of space lattice, unit cell; laws of crystallography – (i) law of constancy of interfacial angles, (ii) law of rational indices (Miller indices) and, (iii) law of symmetry, elementary ideas of symmetry, symmetry elements and symmetry operations. qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of

NaCl, CsCl and KCl. Defects in crystals. Glasses and liquid crystals.

Unit – III: Liquid and Colloidal States

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapor pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water.

Definition of colloids, classification of colloids. Solids in liquids (sols); properties– kinetic, optical and electrical, stability of colloids, protective action; Hardy-Schulze law, gold number. Liquids in liquids (Emulsions): types of emulsions (micelles and reverse micelles), preparation, emulsifier. Liquid in solid (gels): classification, preparation, and properties, general application of colloids.

C. References:

- D. D. Ebbing, *General Chemistry*, 10th Ed., Cengage Learning India Pvt. Ltd., **2013**.
- W. R. Robinson, J. D. Odom and H. F. Holtzclaw, *Essentials of General Chemistry*, 10th Ed., Houghton Mifflin, **1997**.
- P. Atkins, J. d. Paula and K. James, *Physical Chemistry*, 11th Ed., Oxford University Press, **2018**.
- G. W. Castellan, *Physical Chemistry*, Narosa, **2004**.
- K. J. Laidler and J. H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers, **2006**.
- K. L. Kapoor, *A Text Book of Physical Chemistry: States of Matter and Ions in Solution, Vol. 1*, 5th Ed., McGraw-Hill, **2015**.
- S. Alberty, *Physical Chemistry*, 3rd Ed., John Wiley & Sons, Inc., **2003**.
- R. G. Mortimer, *Physical Chemistry*, 3rd Ed., Academic Press, **2008**.
- B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Ed., Vishal Publishing Co., **2018**.
- P. C. Rakshit, *Physical Chemistry*, 7th (Revised) Ed., Sarat Book Distributors, **2012**.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 102/CHE IDMI 104.1	Understand the basic principles and interaction of electromagnetic radiation with matter.	2					1	2		1		2
CHE DMI 102/CHE IDMI 104.2	Apply the concepts of microwave (rotational) spectroscopy techniques.	2		3			1	2	2	1		2
CHE DMI 102/CHE IDMI 104.3	Learn the basic principles and applications of vibrational (IR and Raman) spectroscopy.	2	2	2	3	1			2			1

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

SEMESTER – II

PAPER CODE: CHE DMI 202/ CHE IDMI 204: Chemistry in Daily Life

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the basics of Industrials Chemicals and their Impacts on Environment. Learn the Introduction, history and utilization to agrochemicals and Major Food Component and household chemical.

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

[CHE DMI 202/CHE IDMI 204.1]. Learn the Introduction, General mechanisms that occur after the discharge of a Chemical into the Environment.

[CHE DMI 202/CHE IDMI 204.2]. Understand the basic introduction, history and utilization of agrochemicals.

[CHE DMI 202/CHE IDMI 204.3]. Learn about the Minor Food Components: Vitamins, Minerals, Colorants, Flavors, Food Additives.

[CHE DMI 202/CHE IDMI 204.3]. Learn the properties and uses of household chemicals.

B. SYLLABUS

Unit I: Chemicals in the Environment

Introduction, General mechanisms that occur after the discharge of a Chemical into the Environment, Sources: Point and Non-Point Sources of Pollutants, Atmospheric pollutants (benzene, acid deposits-NO_x and SO_x, Ozone, Radioactive pollutants and their effects, Photochemical Pollutants). Water Pollution and common disinfectants (KMnO4, Chlorination, Ozone, UV light), Industrials Chemicals and their Impacts on Environment.

Unit II Agrochemicals

Demand and supply gap of Food and improving the productivity, Introduction to agrochemicals (insecticides, fungicides, and herbicides), History of agrochemicals and Lead optimization, and Agrochemicals utilized in Modern days and recent markets.

Unit III Food Chemistry

Major Food Components (Major Food Components: Carbohydrates, Lipid, Proteins, and enzymes: Structures, and properties), Minor Food Components: Vitamins, Minerals, Colorants, Flavors, Food Additives etc.

Unit IV Household Chemistry

FUELS: Solid (coal, coke, and charcoal), liquid (kerosene oil, petrol and diesel oil) and gas (LPG and CNG). Non-conventional sources of energy. ACIDS, BASES AND SALTS: Properties and uses of sulphuric acid, hydrochloric acid and nitric acid. Properties and uses of sodium carbonate, sodium bicarbonate, baking powder, boric acid, borax and bleaching powder. Useful Organic Products: Vinegar, Ethyl alcohol, and DRUGS: Antiseptics and disinfectants.

C. Reference Books

- Graham Solomon, T.W., Fryhle, C.B. & Dnyder, S.A. *Organic Chemistry*, John Wiley & Sons (2014).
- McMurry, J.E. *Fundamentals of Organic Chemistry*, 7th Ed. Cengage Learning India Edition, 2013.
- Sykes, P. *A Guidebook to Mechanism in Organic Chemistry*, Orient Longman, New Delhi (1988).
- Finar, I.L. *Organic Chemistry* (Vol. I & II), E.L.B.S.
- Morrison, R.T. & Boyd, R.N. *Organic Chemistry*, Pearson, 2010.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 202/CHE IDMI 204.1	Learn the Introduction, General mechanisms that occur after the discharge of a Chemical into the Environment.	2					1	2		1		2
CHE DMI 202/CHE IDMI 204.2	Understand the basic introduction, history and utilization of agrochemicals	2		3			1	2	2	1		2
CHE DMI 202/CHE IDMI 204.3	Learn about the Minor Food Components: Vitamins, Minerals, Colorants, Flavors, Food Additives.	2	2	2	3	1			2			1
CHE DMI 202/CHE IDMI 204.4	Learn the properties and uses of household chemicals.	1	1						2			3

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

SEMESTER – III

PAPER CODE: CHE DMI 302/ CHE IDMI 304: Basic Analytical Chemistry

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the qualitative and quantitative aspects of analysis for inorganic compounds. Understand the Volumetric Titration and Basic techniques of Spectroscopy.

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

[CHE DMI 302/CHE IDMI 304.1]. Understand the qualitative and quantitative aspects of analysis for inorganic radicals.

[CHE DMI 302/CHE IDMI 304.2]. Learn about the volumetric (redox and acid-base, complex metric) titrations.

[CHE DMI 302/CHE IDMI 304.3]. Learn about the basic techniques of Spectroscopy and its functions.

B. SYLLABUS

Unit – I: Qualitative and quantitative aspects of analysis

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Qualitative Analysis of Inorganic Radicals

Introduction to salt analysis, dry and wet test for acid and basic radicals, Principle and chemistry of qualitative analysis of inorganic salt; chemistry involved in qualitative analysis of mixture containing interfering radicals and insolubles.

Unit - II: Volumetric Titration

Standard solution, primary standard and secondary standard, titration, end point, indicator, concentration of standard solution- moles, Normality, molarity, Molality, parts per million(PPM), volumetric calculation, acid base titration and use of indicators, titration curves for strong acid vs strong base, weak acid with strong base, weak base with strong acid, theory of acid base indicator, Redox titration- titration of Mohr salt against $KMnO_4$, Titration of Oxalic acid against $KMnO_4$, Titration of $FeSO_4$ against $K_2Cr_2O_7$, Iodometric and iodimetric titration, Internal and external indicator, complexometric titration- EDTA titration, Eriochrome black T indicator, complexometric titration curve, direct and back titration, masking and demasking of cations, precaution in volumetric titration.

Unit – III: Basic techniques of Spectroscopy (10Hours)

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law in UV-Visible Spectrometry, Infrared Spectrometry.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and

sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

Reference Books:

- Willard, H. H. *Instrumental Methods of Analysis*, CBS Publishers.
- Skoog & Lerry. *Instrumental Methods of Analysis*, Saunders College Publications, New York.
- Skoog, D.A.; West, D.M. & Holler, F.J. *Fundamentals of Analytical Chemistry 6th Ed.*, Saunders College Publishing, Fort Worth (1992).
- Vogel, A. I. *Vogel's Qualitative Inorganic Analysis 7th Ed.*, Prentice Hall.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 302/CHE IDMI 304.1	Understand the qualitative and quantitative aspects of analysis for inorganic radicals.	2					1	2		1		2
CHE DMI 302/CHE IDMI 304.2	Learn about the volumetric (redox and acid-base, complex metric) titrations.	2		3			1	2	2	1		2
CHE DMI 302/CHE IDMI 304.3	Learn about the basic techniques of Spectroscopy and its functions.	2	2	2	3	1			2			1

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

SEMESTER – IV

PAPER CODE: CHE DMI 402/CHE IDMI 404: Chemical and Phase Equilibria, Solutions and Colligative Properties

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the basic concepts of thermodynamic equilibrium, chemical equilibria in ideal gases, Phase Equilibrium and Phase Transformations, Solutions and Colligative Properties.

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

[CHE DMI 402/CHE IDMI 404.1]. Understand the basic concepts of thermodynamic equilibrium and chemical equilibria in ideal gases.

[CHE DMI 402/CHE IDMI 404.2]. Learn the thermodynamics of phase transition; classification of phases.

[CHE DMI 402/CHE IDMI 404.3]. Learn about basic studies on Solutions and Colligative Properties.

B. SYLLABUS

Unit – I: Chemical Equilibrium

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration; thermodynamic derivation of relations between the various equilibrium constants *Kp*, *Kc* and *Kx*. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Unit – I: Phase Equilibrium and Phase Transformation

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Phase diagrams with applications for one-component systems (water and sulfur) and two component systems involving eutectics, congruent, incongruent melting points and solid solution (lead-silver, FeCl3-H2O and Na-K *etc*.).

Three Component System: Graphical representation of three component system; system of three liquids: having partial miscibility.

Type-I Formation of one pair of partially miscible liquids, **Type-II** Formation of two pairs of partially miscible liquids, **Type-III** Formation of three pairs of partially miscible liquids

Stability of phases; Clapeyron equation; Clasius-Clapeyron equation and its applications to solid-liquid, liquid-vapor and solid-vapor equilibria. Thermodynamics of phase transition; classification of phases - bubbles, cavities and droplets-Kelvin equation.

Unit – III: Solutions and Colligative Properties

The chemical potential of liquids; ideal solutions; lowering of vapor pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions.

Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapor pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated, and associated solutes in solution.

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), vapor pressure-composition and temperature-composition curves of ideal and non-ideal solution; distillation of solution, Lever rule, azeotropes. Partial miscibility of liquids, CST, miscible pairs, Immiscibility of liquids – Principle of steam distillation.

Nernst distribution law: its derivation and applications.

References Books:

- S. Alberty, *Physical Chemistry*, 3rd Ed., John Wiley & Sons, Inc., **2003**.
- P. Atkins, J. d. Paula and K. James, *Physical Chemistry*, 11th Ed., Oxford University Press, **2018**.
- G. W. Castellan, *Physical Chemistry*, Narosa, **2004**.
- K. L. Kapoor, *A Text Book of Physical Chemistry: Thermodynamics and Chemical Equilibrium, Vol. 2*, 5th Ed., MsGraw-Hill, **2015**.
- K. L. Kapoor, *A Text Book of Physical Chemistry: Applications of Thermodynamics, Vol. 3*, 5th Ed., McGraw-Hill, **2015**.
- K. J. Laidler and J. H. Meiser, *Physical Chemistry*, 2nd Ed., CBS Publishers, **2006**.
- R. G. Mortimer, *Physical Chemistry*, 3rd Ed., Academic Press, **2008**.
- B. R. Puri, L. R. Sharma and M. S. Pathania, *Principles of Physical Chemistry*, 47th Ed., Vishal Publishing Co., **2018**.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 402/CHE IDMI 404.1	Understand the basic concepts of thermodynamic equilibrium and chemical equilibria in ideal gases.	2					1	2		1		2
CHE DMI 402/CHE IDMI 404.2	Learn the thermodynamics of phase transition; classification of phases.	2		3			1	2	2	1		2
CHE DMI 402/CHE IDMI 404.3	Learn about basic studies on Solutions and Colligative Properties.	2	2	2	3	1			2			1

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

SEMESTER – V

PAPER CODE: CHE DMI 502/ CHE IDMI 504: Advanced Analytical Chemistry

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the classification, principle and efficiency of separation techniques, gravimetric analysis and basic principle of instrumentation techniques of thermal and electroanalytical analysis.

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

[CHE DMI 502/CHE IDMI 504.1]. Understand the classification, principle and efficiency of the chromatographic techniques.

[CHE DMI 502/CHE IDMI 504.2]. Learn the basic principle of gravimetry, preparation of solution, precipitation, condition for analytical precipitation.

[CHE DMI 502/CHE IDMI 504.3]. Learn about the basic principle of instrumentation techniques of thermal and electroanalytical analysis.

B. SYLLABUS

Unit – I: Separation techniques:

Solvent extraction: Classification, principle and efficiency of the technique. Distribution Coefficient, distribution ratio, percent extracted.
Mechanism of extraction: extraction by solvation and chelation.
Technique of extraction: batch, continuous and counter current extractions.
Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

***Ion-exchange*:** Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Chromatography: Classification, principle and efficiency of the technique.
Mechanism of separation: adsorption, partition & ion exchange.
Development of chromatograms: frontal, elution and displacement methods.
Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Gas Chromatography: retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Unit – II: Gravimetric analysis:

Basic principle of gravimetry, preparation of solution, precipitation, condition for analytical precipitation, saturation, supersaturation, nucleation, von weimarn ratio, digestion of the precipitate,

Ostwald ripening, colloidal, peptization, impurities in precipitates, occlusion, inclusion, surface adsorption, postprecipitation, washing and filtering the precipitates, drying the precipitate, gravimetric calculation

Unit – III: Thermal and Electroanalytical analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture. 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.

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK_a values.

C. Reference Books:

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

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 502/CHE IDMI 504.1	Understand the classification, principle and efficiency of the chromatographic techniques.	2					1	2		1		2
CHE DMI 502/CHE IDMI 504.2	Learn the basic principle of gravimetry, preparation of solution, precipitation, condition for analytical precipitation	2		3			1	2	2	1		2
CHE DMI 502/CHE IDMI 504.3	Learn about the basic principle of instrumentation techniques of thermal and electroanalytical analysis.	2	2	2	3	1			2			1

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

SEMESTER – VI

PAPER CODE: CHE DMI 602/ CHE IDMI 605: Organic Spectroscopy

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the Basics of Organic Spectroscopy and Ultraviolet Spectroscopy and fundamentals of Infrared Spectroscopy, Nuclear Magnetic Resonance and Mass Spectroscopy.

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

[CHE DMI 602/CHE IDMI 605.1]. Understand the basics of Organic Spectroscopy and Ultraviolet Spectroscopy.

[CHE DMI 602/CHE IDMI 605.2]. Learn the fundamentals of Infrared Spectroscopy and important group frequencies for the common functional groups.

[CHE DMI 602/CHE IDMI 605. 3]. Learn about the Nuclear Magnetic Resonance and Mass Spectroscopy of organic compounds. .

[CHE DMI 602/CHE IDMI 605.4]. Determination of molecular formula of organic compounds based on Mass Spectroscopy.

B. SYLLABUS

Unit I: Basics of Organic Spectroscopy and Ultraviolet Spectroscopy

Electromagnetic radiations: Types of molecular energy and molecular 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.

Unit II: Infrared Spectroscopy

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

Unit III: 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). 13C NMR, Heteronuclear coupling, Chemical shifts, coupling constant,

Unit IV: Mass Spectrometry

Molecular ion peak, base peak, isotopic abundance, 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

References:

- Spectroscopy of Organic Compounds, JOHN WILEY, 2001-By Bessler and Silverstein

- Introduction to Spectroscopy, 3rd Edition, Thomson, 2007-By D. C. Pavia, G. M. Lampman, G. S. Kriz:
- Organic Spectroscopy, III Edition-By William Kemp

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 602/CHE IDMI 605.1	Understand the basics of Organic Spectroscopy and Ultraviolet Spectroscopy.	2					1	2		1		2
CHE DMI 602/CHE IDMI 605.2	Learn the fundamentals of Infrared Spectroscopy and important group frequencies for the common functional groups.	2		3			1	2	2	1		2
CHE DMI 602/CHE IDMI 605.3	Learn about the Nuclear Magnetic Resonance and Mass Spectroscopy of organic compounds. .	2	2	2	3	1			2			1
CHE DMI 602/CHE IDMI 605.4	Determination of molecular formula of organic compounds based on Mass Spectroscopy.	1	1						2			3

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

CHE DMI 102/ CH IDMI 103: IT Skill for Chemists

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the Fundamentals, mathematical functions, polynomial expression, algebraic operations on real scalar variables, introductory writing activities & Handling numeric data, Numeric modeling & Statistical Analysis

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

[CHE DMI 102/ CH IDMI 103.1]. Understand the basics of Learn the Fundamentals, mathematical functions, polynomial expression

[CHE DMI 102/ CH IDMI 103.2]. Learn the fundamentals of algebraic operations on real scalar variables, introductory writing activities

[CHE DMI 102/ CH IDMI 103. 3]. Learn about the Nuclear Magnetic Resonance and Mass Spectroscopy of organic compounds. .

[CHE DMI 102/ CH IDMI 103.4]. Learn the handling numeric data, Numeric modeling & Statistical Analysis

B. SYLLABUS

Unit – I: Mathematics

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms).Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

Unit – II: Introductory writing activities & Handling numeric data

Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs. Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

Unit – III: Numeric modeling & Statistical Analysis

Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration-time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pK_a of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Statistical Analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The *t* test. The *F* test.

Presentation: Presentation graphics

Reference Books:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical calculations. 2nd Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical chemistry on a Microcomputer.* Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 102/ CH IDMI 103.1	Understand the basics of Learn the Fundamentals, mathematical functions, polynomial expression**.**	2					1	2		1		2
CHE DMI 102/ CH IDMI 103.2	Learn the fundamentals of algebraic operations on real scalar variables, introductory writing activities.	2		3			1	2	2	1		2
CHE DMI 102/ CH IDMI 103.4	Learn the handling numeric data, Numeric modeling & Statistical Analysis.	2	2	2	3	1			2			1

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

PAPER CODE: CHE DMI 202/ CHE IDMI 204: Green Methods in Chemistry

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the basic Introduction to green chemistry and principles and process, examples of green synthesis/ reactions

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

[CHE DMI 202/ CHE IDMI 204.1]. Learn the basic Introduction and limitation of green chemistry.
[CHE DMI 202/ CHE IDMI 204.2]. Learn the basic principles, examples of green chemistry.
[CHE DMI 202/ CHE IDMI 204.3]. Learn the basic examples of green synthesis/ reactions.
[CHE DMI 202/ CHE IDMI 204.4]. Learn the basic future trends in green chemistry.

B. SYLLABUS

Unit – I: Short Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Unit – II: Principles

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples. Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals: green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Unit – III: Examples of Green Synthesis/ Reactions

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, citral, ibuprofen, paracetamol, furfural.
2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole acid), Oxidation (of toluene, alcohols).
3. Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation.
4. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine

derivatives; benzimidazoles.

5. Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizaro reaction, Strecker synthesis, Reformatsky reaction.

Unit – IV: Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistry in sustainable development.

Reference Books:

1. Manahan S.E. (2005) Environmental Chemistry, CRC Press
2. Miller, G.T. (2006) Environmental Science 11th edition. Brooks/Cole
3. Mishra, A. (2005) Environmental Studies. Selective and Scientific Books, New

Reference Books:

- McQuarrie, D. A. Mathematics for Physical Chemistry University Science Books (2008).
- Mortimer, R. Mathematics for Physical Chemistry. 3rd Ed. Elsevier (2005).
- Steiner, E. The Chemical Maths Book Oxford University Press (1996).
- Yates, P. Chemical calculations. 2nd Ed. CRC Press (2007).
- Harris, D. C. *Quantitative Chemical Analysis*. 6th Ed., Freeman (2007) Chapters 3-5.
- Levie, R. de, *How to use Excel in analytical chemistry and in general scientific data analysis*, Cambridge Univ. Press (2001) 487 pages.
- Noggle, J. H. *Physical chemistry on a Microcomputer.* Little Brown & Co. (1985).
- Venit, S.M. *Programming in BASIC: Problem solving with structure and style*. Jaico Publishing House: Delhi (1996).

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 202/ CHE IDMI 204.1	Learn the basic Introduction and limitation of green chemistry.	2					1	2		1		2
CHE DMI 202/ CHE IDMI 204.2	Learn the basic principles, examples of green chemistry.	2		3			1	2	2	1		2
CHE DMI 202/ CHE IDMI 204.3	Learn the basic examples of green synthesis/ reactions.	2	2	2	3	1			2			1
CHE DMI 202/ CHE IDMI 204.4	Learn the basic future trends in green chemistry.	2	2	2	3	1			2			1

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

PAPER CODE: CHE DMI T 302/ CH IDMI 304: Basic of Nanomaterials

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn the basic Introduction, Properties, Synthesis, and Characterization & Applications of Nanomaterials.

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

[CHE DMI T 302/ CH IDMI 304.1]. Learn the basic introduction and classification of nanomaterials.
[CHE DMI T 302/ CH IDMI 304.2]. Learn the basic properties and synthesis of nanomaterials.
[CHE DMI T 302/ CH IDMI 304.3]. Learn the basic characterization and applications of nanomaterials.

B. SYLLABUS

Unit – I: Introduction and Classification

What is nanotechnology?; Why nano? Classification of nanostructures, nanoscale architecture; summary of the electronic properties of atoms and solids; the isolated atom, bonding between atoms, giant molecular solids, the free electron model and energy bands of crystalline solids, periodicity of crystal lattices; electronic conduction; effects of the nanometre length scale, changes to the system total energy, changes to the system structure; how nanoscale dimensions affect properties. (electronic conduction, system classification confined to one, two or three dimension and their effect on properties).

Unit – II: Properties & Synthesis of Nanomaterials

Properties: Introductory discussion of size and shape dependable properties of nanomaterials like melting point, magnetism, optical, conductivity (conductor and semi-conductivity), catalytic and electrochemical aspect.

Synthesis: Common methods of top down and bottom approaches of the preparation of nanomaterials. Special interest on the synthesis of metal nanoparticles, metal oxides, and carbon nanotube (CNT) *etc*. A brief discussion of biological synthesis of nanomaterials.

Unit – IV: Characterization & Applications of Nanomaterials

Characterization: A brief historical overview of common instrumental techniques used for characterization of nanomaterials such as, X-ray diffraction, electron microscopy (SEM, TEM, including EDX technique), XPS with respect to working principle, instrumentation and applications. Differential scanning calorimeter (DSC), Thermogravimetric / Diffferential (TG/DTA), UV-Visible Spectrophotometer, and FTIR –Principle and Applications.

Applications: Use of nanomaterials in daily life with examples (solar cell, GMR read heads, NEMS goniometers, health care, energy materials, *etc*). Societal aspects of nanotechnology: health, environment, hype and reality.

Reference Books:

- Hornyak, G. L.; Moore, J. J.; Tibbals, H. F. and Dutta, J. *Fundamentals of Nanotechnology*, CRC Press, 2009.
- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).
- Cao, G. *Nanostructures and Nanomaterials Synthesis, Properties and Appli-cations*, Imperial College Press, London, 2004.
- Klabunde, K. J. *Nanoscale materials in Chemistry*, Wiley-Interscience, (2001).
- Knauth, P. and Schoonman, J. *Nanostructured Materials: Selected Synthesis Methods, Properties and Applications*, Kluwer Academic Publishers, New York, (2002).
- Cullity, B. D., *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, **1959**.
- Williams, D. B. and Carter C. B., *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, **1996**.
- Brugel W., in *Introduction to Infrared Spectroscopy*, John Wiley and Sons, New York, **1962**. S. Hüfner, in *Photoelectron Spectroscopy: Principles and Applications*, Springer-Verlog, Germany, **1995**.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI T 302/ CH IDMI 304.1	Learn the basic introduction and classification of nanomaterials.	2					1	2		1		2
CHE DMI T 302/ CH IDMI 304.2	Learn the basic properties and synthesis of nanomaterials.	2		3			1	2	2	1		2
CHE DMI T 302/ CH IDMI 304.3	Learn the basic characterization and applications of nanomaterials.	2	2	2	3	1			2			1

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

PAPER CODE: CHE DMI 402/ CHE IDMI 404: Crystalline Materials and Properties

Full Mark 50 (30 + 20)

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

[CHE DMI 402/ CHE IDMI 404.1]. Understand the basics introduction, bonding and crystal structure of the materials.

[CHE DMI 402/ CHE IDMI 404.2]. Learn the determination of crystal structure by electron microscopic techniques.

[CHE DMI 402/ CHE IDMI 404.3]. Understand the thermal, electrical and magnetic properties of solids.

B. SYLLABUS

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Unit – I: Introduction, Bonding & Crystal structure of the Materials

Introduction: Crystalline and non-crystalline solids; space lattice and primitive and non-primitive lattice, crystal structure, unit cell, symmetry in crystal, seven crystal system, Bravais lattice, a qualitative ideas of point and space group; crystal planes and Miller indices, reciprocal lattice.

Cubic lattice: lattice point in cubic crystals, coordination number, Packing density, separation between crystal planes

Bonding and Crystal Structure of Crystalline Materials

Closed packed structure- hcp and ccp, packing efficiency, voids, limiting radius ratio; description of solid structure of rack salt (NaCl), Wurzite and zinc blend of ZnS, Fluoride (CaF_2) and antifluoride (Na_2O), Rutile (TiO_2).

Bonding between atoms in solid: ionic bonds, covalent bonds, metallic bonds, van der Waals bonds; cohesive energy of an ionic crystal, Madelung constant and lattice energy.

Unit – II: Determination of Crystal Structure

X-ray diffraction by crystal, Bragg's law, a simple description of rotating crystal method and powder pattern methods. Analysis of powder pattern of simple cubic systems.

A brief overview of determination of crystal structure by electron microscope (TEM, SAED, and HRTEM)

Unit – III: Thermal, Electrical and Magnetic Properties of Solids

Thermal Properties: Specific heat of solids, classical theory – Dulong-Petit's law, Einstein-Debye theory, vibrational modes of one dimensional lattice – dispersion relation and Brillouin zones.

Electronic Properties: Free electron theory of metals; solution of one dimensional Schrödinger equation in constant potential; density of state; Fermi energy; Energy band in a solid, explanations of Kronig-Penney model (without derivation), refinement of simple band formation in solid, *k*-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, *p*-*n* junctions. Hall effect- definition, Hall potential Hall coefficient.

Superconductivity- qualitative discussion, critical temperature, Meissner effect, and Josephson Tunnelling.

Magnetic Properties of Solids: Concept of dia- para- and ferro- magnetism; magnetic moment due to orbital and spin motion of electron, effect of temperature, Langevin's theory of dia- and para- magnetism; Curie-Weiss law, qualitative description of ferro-magnetism (magnetic domains), B-H curve, hysteresis loop, retentivity, coercivity, hysteresis loss, soft and hard magnets.

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.
- L. V. Azaroff Introduction to Solid, Tata Mcgraw Hill
- Cullity, B. D., *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, **1959**.
- Williams, D. B. and Carter C. B., *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, **1996**.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 402/ CHE IDMI 404.1	Understand the basics introduction, bonding and crystal structure of the materials.	2					1	2		1		2
CHE DMI 402/ CHE IDMI 404.2	Learn the determination of crystal structure by electron microscopic techniques.	2		3			1	2	2	1		2
CHE DMI 402/ CHE IDMI 404.3	Understand the thermal, electrical and magnetic properties of solids.	2	2	2	3	1			2			1

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

PAPER CODE: CHE DMI 502/ CHE IDMI 504: Inorganic Materials of Industrial Importance

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the inorganic silicate, fertilizer, surface coatings batteries, alloys materials and their industrial importance.

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

[CHE DMI 502/ CHE IDMI 504.1]. Understand the basics inorganic silicate materials and their industrial importance.

[CHE DMI 502/ CHE IDMI 504.2]. Learn the inorganic fertilizer, surface coatings materials and their industrial importance.

[CHE DMI 502/ CHE IDMI 504.3]. Learn the inorganic batteries, alloys materials and their industrial importance.

B. SYLLABUS

Unit – I: Silicate Industries

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.

Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.

Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

Unit – II: Fertilizer & Surface Coatings

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

Unit – III: Batteries & Alloys

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer

cell.

Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

Unit – IV: Catalysis & Chemical explosives

General principles and properties of catalysts, homogenous catalysis (catalytic steps and examples) and heterogenous catalysis (catalytic steps and examples) and their industrial applications, Deactivation or regeneration of catalysts.

Phase transfer catalysts, application of zeolites as catalysts.

Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

Reference Books:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics*, Wiley Publishers, New Delhi.
- J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.
- P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
- B. K. Sharma: *Engineering Chemistry*, Goel Publishing House, Meerut

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 502/ CHE IDMI 504.1	Understand the basics inorganic silicate materials and their industrial importance.	2					1	2		1		2
CHE DMI 502/ CHE IDMI 504.2	Learn the inorganic fertilizer, surface coatings materials and their industrial importance.	2		3			1	2	2	1		2
CHE DMI 502/ CHE IDMI 504.2	Learn the inorganic batteries, alloys materials and their industrial importance.	2	2	2	3	1			2			1

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

PAPER CODE: CHE DMI 602/ CHE IDMI 605: Basics of Drug Design & Medicinal Chemistry

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the basic concepts of drug design, physiochemical factors, molecular modeling, ligand design concept and herbal medicine.

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

[CHE DMI 602/ CHE IDMI 605.1]. Understand the basics concepts of drug design, physiochemical factors.

[CHE DMI 602/ CHE IDMI 605.2]. Learn the concept of structure of drug molecules and its optimization. **[CHE DMI 602/ CHE IDMI 605.3].** Learn the classification and applications of drugs.

[CHE DMI 602/ CHE IDMI 605.4]. Understand the herbal medicine/herbal drug and its importance in daily life.

B. SYLLABUS

Unit – I: Basic Concept of Drug Design & Physiochemical Factors

Introduction; Basics of drug design; analog and Prodrug; Cocept of lead; Factors governing drug design; Rational approach to drug design.

Physical-Chemical factors and biological activities; Factors governing ability of drug to reach active site.

Unit – II: Molecular Modeling & Ligand Design Concept

Concept of structure of drug molecules and its optimization; Molecular modeling and drug design; Basic concept of Protein and its structure; Structure based drug design; Ligand receptor recognition; Active site of a target molecules; Characterization of site and design of ligands.

Unit – III: Types of Drugs

Concept of Analgesics drug; Synthesis and use of analgesics drugs: Paracetamol, Phenacetine, Acetanilide, Aspirin, Salol, Cinchophene, and Phenazone.

Antimalerial Drugs: Synthesis and use of Chloroquine phosphate.

Antibacterial Drugs & Properties:

Sulphonamide drugs: Synthesis and use of Sulphonamide drugs: Sulphanilide, Sulphapyridine, Sulphathiazole, Sulphadiazine, Antibacterial properties.

Concept of Antibiotics with its application.

Unit – IV: Herbal medicine

Herbal Drug: Its importance

Ethanobotanical survey methods; introduction to ayurveda, pharmacopia; plants as source of drugs; Indian medicinal plants and uses - Tulasi, Neem, Pili, Mango, Sarpagandhi, Gulbakavali, Shyma Haldi, Vanchana, Safed Musli, Aswagandha, Satavar, Pipalendi, Digitalis, Senna, Clove, Cardamom, Plantago, *Artemisia annua*, *Coleus forskoli*, Aloe

Patal Kumhda, Banpyaz.

Reference Books:

- Asutosh Kar, *Medicinal Chemistry*, New Age Publication.
- P. D. Sethi, Dilip Charegaonkar: *Identification of Drugs and Pharmaceutical Formulations by Thin Layer Chromatography* –2nd Edition.
- G.E. Trease, W.C. Evans: *Pharmacognosy*, ELBS.
- Varro E.Tyler, Lynn. R.Brady, James E.Robbers: Pharmacognosy.
- T.E. Wallis: Text Book of Pharmacognosy, CBS Pub. Delhi.
- Kirthikar, Basu: Indian Medicinal Plants.
- K.M. Nalkarni: Indian Meteria Medica
- W. Dymock: Pharmacographia Indica

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE DMI 602/ CHE IDMI 605.1	Understand the basics concepts of drug design, physiochemical factors.	2					1	2		1		2
CHE DMI 602/ CHE IDMI 605.2	Learn the concept of structure of drug molecules and its optimization.	2		3			1	2	2	1		2
CHE DMI 602/ CHE IDMI 605.3	Learn the classification and applications of drugs.	2	2	2	3	1			2			1
CHE DMI 602/ CHE IDMI 605.4	Understand the herbal medicine/herbal drug and its importance in daily life.	2	2	2	3	1			2	2		1

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

Vocational Paper in Chemistry:

Semester	Paper Code	Course Title	Credit
I	CHE VOT 105	Basic Concepts of Physical Chemistry Experiments, Energy, and Environment	02
	CHE VOP 106	Vocational Chemistry Practical – I	02
II	CHE VOT 205	Cosmetics, Perfumes, & Pharmaceutical Chemistry	02
	CHE VOP/I 206	Vocational Chemistry Practical – II /Internship (Industrial visit)	02
III	CHE VOT 305	Cement, Extraction of Ores, Pesticides & Fuel Chemistry	02
	CHE VOP 306	Vocational Chemistry Practical – III	02
IV	CHE VOT 405	Techniques of Instrumental Analysis (Principles and Applications of X-ray diffraction, FT-IR, UV, GCMS, LCMS etc.)	02
	CHE VOP/I 406	Hands Training on Instrument	02

PAPER CODE: CHE VOT 105: Basic Concepts of Physical Chemistry Experiments, Energy, and Environment

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the safety measures in chemical laboratory and experiment execution, treatment of experimental data, energy and environment.

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

[CHE VOT 105.1]. Understand the basic safety measures in chemical laboratory and experiment execution.

[CHE VOT 105.2]. Learn the significant figures, accuracy and precision in calculations and error in data and results.

[CHE VOT 105.3]. Learn the basic introduction, concepts of energy and environment.

B. SYLLABUS

Unit I- Safety Measures in Chemical Laboratory and Experiment Execution

Introduction to chemical laboratory: general guidelines, cleanness, reagents, glasswares, and equipments; safety symbols and regulations in chemical laboratory. Materials Safety Data Sheet (MSDS). Globally CAS registry number. Global overview of chemical regulations in India. Fundamentals units of measure. Analytical balance and weights: general purpose chemical balance, electronic balance, analytical weight box and classification, calibration of weights and handling of electronic balance. Handling of laboratory apparatus and hazardous chemicals. Calibration of glassware (pipette, burette, etc.).

Types of solutions: mole and mole concept, equivalent weight, formula weight. Expression of concentration, molarity (M), molality (m), mole fraction, normality (N); weight, volume, and weight-to-volume ratios; parts per million (ppm), parts per billion (ppb).

Preparation of an experiment: Literature Work; Execution of an Experiment (general advice, data collection, bias, safety); Recording of Experimental Data (what to record, computer files and disks); Reporting of works (Style, format, tables, figures,) in term of Introduction, Experimental Methods, Result and Discussion. Ethics, References.

Unit –II: Treatment of Experimental Data

Significant figures, accuracy and precision in calculations. Uncertainties (error) in Data and Results, classification of errors, minimizations of errors, distribution of random errors, propagation of error. Reliability of Results, Confidence Interval, Rejection of data (t-test, F-test, and Q-test), Mean and Standard Deviations, Correlation and Regression,

Use of Computer: Excel spread sheet, data entry and manipulation, formula entry and addressing, significance test, Graph plotting, curve fitting (linear and non-linear), and its analysis (including origin software), and advanced spreadsheet tools.

Microsoft power point presentation, Molecule design and its properties determination using computational softwares, Introduction of various computational softwares for chemical sciences.

Unit III- Energy and Environment

Energy, Solar energy, Coal, petroleum and natural gas, Hydro-power, wind power, ocean energy, geothermal energy, Nuclear energy: Fission & Fusion, Fuel cells, & Battery.
Ecosystem, Environmental and its segments, Green house effect, Global warming, Air pollution, Water pollution, Soil pollution, Industrial waste, Control measures of environmental pollution. Plastic pollutants and remedies.

Reference Books:

- D. Harvey, *Modern Analytical Chemistry*, Mc-Graw Hill, **2000**.
- S. M. Khopkar, *Environmental Pollution Analysis* New Age International, **2020**.
- S. E. Manaham, *Environmental Chemistry*, 9th Ed., CRC Press, **2009**.
- P. Patnaik, *Dean's Analytical Chemistry Handbook*, 2nd Ed., Mc-Graw Hill, **2004**.
- A. M. Halern and G. C. McBane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd Ed., W. H. Freeman and Company, **2006**.
- C. W. Garland, J. W. Nibler, and D. P. Shoemaker, *Experiments in Physical Chemistry*, 8th Ed., McGraw-Hill, **2003**.
- R. de Levie, *How to use excel® in analytical chemistry and in general scientific data analysis*, Cambridge University Press, **2004**.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE VOT 105.1	Understand the basic safety measures in chemical laboratory and experiment execution.	2					1	2		1		2
CHE VOT 105.2	Learn the significant figures, accuracy and precision in calculations and error in data and results.	2		3			1	2	2	1		2
CHE VOT 105.3	Learn the basic introduction, concepts of energy and environment.	2	2	2	3	1			2			1

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

CHE VOP 106: Vocational Chemistry Practical – 1

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

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the basic concepts of preparation of standard solutions, and determination of COD and BOD and etc.

SYLLABUS

1. Calibration of weights and glasswares.
2. Preparation of solutions for given concentrations.
3. Measurement of pH of tape water.
4. Measurement of conductivity of given unknown solution.
5. Determination of Biological Oxygen Demand (BOD)
6. Determination of Chemical Oxygen Demand (COD)
7. Measurement of chloride, sulfate and salinity of water samples by simple titration methods ($AgNO_3$ and potassium chromate)
8. Programming of computer applications.
9. Graph plotting with data provided.
10. ***Some others experiments in the class if permit.***

Reference Books:

- A. J. Elias, *A Collection of Interesting General Chemistry Experiments*, Revised Ed., University Press, **2007**.
- R. Brent, *The Golden Book of Chemistry Experiments*, Golden Press, **1960**.
- D. Harvey, *Modern Analytical Chemistry*, Mc-Graw Hill, **2000**.
- A. M. Halern and G. C. McBane, *Experimental Physical Chemistry: A Laboratory Textbook*, 3rd Ed., W. H. Freeman and Company, **2006**.
- G. H. Jeffery, J. Bassett, J. Mendham, and R. C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th Ed., John Wiley & Sons, **1989**.
- C. W. Garland, J. W. Nibler, and D. P. Shoemaker, *Experiments in Physical Chemistry*, 8th Ed., McGraw-Hill, **2003**.
- P. C. Kamboj, *University Practical Chemistry*, 1st Ed., Vishal Publishing, **2013**.
- https://www.originlab.com

PAPER CODE: CHE VOT 205: Cosmetics, Perfumes & Pharmaceutical Chemistry

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the introduction, synthesis of cosmetics, perfumes and drugs & pharmaceuticals.

A. Course Outcomes: At the end of the course, students will be able to
[CHE VOT 205.1]. Understand the basic introduction, synthesis of cosmetics, perfumes
[CHE VOT 205.2]. Learn the synthesis of cosmetics and perfumes.
[CHE VOT 205.3]. Understand the basic introduction, synthesis of drugs and pharmaceuticals.

B. SYLLABUS

Unit – I: Introduction of Cosmetics & perfumes chemistry

History of Cosmetics & perfumes chemistry, a general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

Unit – II: Synthesis procedure

1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

Unit – III: Drugs & Pharmaceuticals

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation: Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

Reference Books:

- E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
- P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- B.K. Sharma: *Industrial Chemistry,* Goel Publishing House, Meerut.
- G.L. Patrick: Introduction to *Medicinal Chemistry*, *Oxford University* Press, UK.
- Hakishan, V.K. Kapoor: *Medicinal and Pharmaceutical Chemistry,* Vallabh Prakashan, Pitampura, New Delhi.
- William O. Foye, Thomas L., Lemke , David A. William: *Principles of Medicinal Chemistry*, B.I. Waverly
- Pvt. Ltd. New Delhi.

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

COURSES	STATEMENT	CORRELATION WITH PROGRAM OUTCOMES							CORRELATION WITH PROGRAMSPECIFIC OUTCOMES			
		PO1	PO2	PC3	PC4	PC5	PC6	PO7	PSO 1	PSO 2	PSO 3	PSO 4
CHE VOT 205.1	Understand the basic introduction, synthesis of cosmetics, perfumes.	2					1	2		1		2
CHE VOT 205.1	Learn the synthesis of cosmetics and perfumes.	2		3			1	2	2	1		2
CHE VOT 205.1	Understand the basic introduction, synthesis of drugs and pharmaceuticals.	2	2	2	3	1			2			1

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

PAPER CODE: CHE VOP/I 206: Vocational Chemistry Practical – II

Full Mark 50

Course Objectives: The learners are Able to: Learn about synthesis and characterization of drugs.

C. SYLLABUS

(a) Drawing of different organic molecules using ChemDraw and ChemSketech software.
(b) Synthesis and characterization of following drugs:

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

PAPER CODE: CHE VOT 305: Cement & Ores, Pesticide & Fuel Chemistry

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the basic history, classification and synthesis and applications of cement, pesticide and fuels.

A. Course Outcomes: At the end of the course, students will be able to
[CHE VOT 305.1]. Understand the basic history, classification and applications of cement and ores.
[CHE VOT 305.2]. Learn about the classification and synthesis and applications of pesticides.
[CHE VOT 305.3]. Review of energy sources (renewable and non-renewable).

B. SYLLABUS

Unit – I: Cement & Extraction of Ores

History of binding materials and Cement, Classification of Cement Binders, Lime as Binder, cement and its importance in construction, History of Cement manufacturing process, material composition of cement, various unit operation of cement manufacture in India, Sources of cement raw materials, Calcareous Materials: Source of Lime, Limestone, Chalk, Marl.

Argillaceous raw materials: Source of Silica, Alumina, Iron Oxide, Shale and effect of coalash.

Alternate Raw Materials: Industrial waste, types of industrial waste use as alternative raw materials for cement manufacture: fly ash, blast furnace slag, LD slag, red mud, lime sludge, phosphogypsum, jerosite, lead and zinc slag, kimberlight rejects, marble slurry, mines rejects, cement kiln dust

Type of Cements: Ordinary Port Land Cement with different grade, Portland Pozzolana Cement, Portland Slag Cement, Ordinary & Rapid Hardening Portland cement, Sulphate Resisting Portland cement, White Portland cement, Coloured Portland cement, Water Repellent and Hydrophobic Portland cement , Masonry cement, Super Sulphate cements, High Early Strength cement.

Additives and Gypsum: Origin and occurrences, distribution/ availability in India, Physical and Chemical Characteristics of various additives such as Bauxite, Iron Ore, Laterite, and gypsum.

Extraction of Ores: Bauxite, Iron, etc.

Unit – II: Pesticide Chemistry & Preparation Procedure

General introduction of Chemical toxicology and pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Unit –III: Fuel Chemistry

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value.
Coal: Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications.

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants: Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants.

Properties of lubricants (viscosity index, cloud point, pore point) and their determination.
Reference Books:

- Norms for limestone exploration for cement manufacture : NCCBM
- Text Book of Geology : P K Mukherjee
- Geology of India and Burma : MS Krishnan, CBS Publisher and Distributer, Delhi
- Chemistry of Cement and Concrete: F M Lea, Arnold, London
- Cement Industry Data Book, CAM, NewDelhi
- World Cement Directory : CEMBUREAU
- Cement Data Book: W. H Duda,VerlagG mBh,Berlin.
- Assessment of utilization of Industrial solid Wastes in cement manufacturing, CPCB
- R. Cremlyn: *Pesticides*, John Wiley.
- E. Stocchi: *Industrial Chemistry*, Vol -I, Ellis Horwood Ltd. UK.
- P.C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- B.K. Sharma: *Industrial Chemistry*, Goel Publishing House, Meerut.

A. 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
CHE VOT 305.1	Understand the basic history, classification and applications of cement and ores.	2					1	2		1		2
CHE VOT 305.2	Learn about the classification and synthesis and applications of pesticides	2		3			1	2	2	1		2
CHE VOT 305.3	Review of energy sources (renewable and non-renewable).	2	2	2	3	1			2			1

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

PAPER CODE: CHE VOP 306: Vocational Chemistry Practical – III

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the basic analysis of ores, felspar, bauxite, rocks. Chromatographic separation of chemical.

C. SYLLABUS

I. (i) Analysis of Ores: Felspar, bauxite, Rocks available in that region (At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session)

(ii) Determination of composition of dolomite (by complexometric titration).
(iii) Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
(iv) Analysis of Cement: Determination of density, Determination of specific surface, Determination of setting time, Determination of soundness test by Le Chatelier Autoclave, Determination of compressive strength, Determination of drying shrinkage
(v) Preparation of pigment (zinc oxide).
(vi) Analysis of Soil sample, animal feeds, soil micronutrients, milk powder for Ca, Fe and P content.
(vii) Estimation of calcium, magnesium, phosphate, nitrate in fertilizer
(viii) Determination of pH of soil.

II. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

i. Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}.
ii. Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.

(b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.

(c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

Reference Books:

- E. Stocchi: *Industrial Chemistry*, Vol-I, Ellis Horwood Ltd. UK.
- R. M. Felder, R. W. Rousseau: *Elementary Principles of Chemical Processes*, Wiley Publishers, New Delhi.
- W. D. Kingery, H. K. Bowen, D. R. Uhlmann: *Introduction to Ceramics,* Wiley Publishers, New Delhi.
- J. A. Kent: Riegel's *Handbook of Industrial Chemistry*, CBS Publishers, New Delhi.

- P. C. Jain, M. Jain: *Engineering Chemistry*, Dhanpat Rai & Sons, Delhi.
- R. Gopalan, D. Venkappayya, S. Nagarajan: *Engineering Chemistry*, Vikas Publications, New Delhi.
- B. K. Sharma: *Engineering Chemistry*, Goel Publishing House.
- Mikes, O. & Chalmes, R.A. Laboratory Hand Book of Chromatographic & Allied Methods, Elles Harwood Ltd. London.
- Ditts, R.V. Analytical Chemistry – Methods of separation.
- Vogel, Arthur I: A Test book of Quantitative Inorganic Analysis (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman.

PAPER CODE: CHE VOT 405: Techniques of Instrumental Analysis

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the basic fundamental laws of spectroscopy and selection rules. Basic introduction and applications of X-Ray Diffraction, Mass spectroscopy & Chromatography.

A. Course Outcomes: At the end of the course, students will be able to
[CHE VOT 405.1]. Learn about the basic fundamental laws of UV, FT-IR spectroscopies and selection rules.
[CHE VOT 405.2]. Learn the basic introduction and applications of X-Ray Diffraction.
[CHE VOT 405.3]. Basic introduction and applications of Mass spectroscopy & Chromatography.

B. SYLLABUS

Unit – I: Basic Spectroscopy

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Fluorescence Spectroscopy: Basic principles of fluorescence spectrophotometer, Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

NMR spectroscopy: Principle, Instrumentation, Chemical shift, Factors affecting chemical shift, Spin-coupling, Applications: ^{1}H-NMR spectroscopy and 13C-NMR

Unit – II: X-Ray Diffraction

Crystalline and non-crystalline solids; space lattice and primitive and non-primitive lattice, crystal structure, unit cell, symmetry in crystal, seven crystal system, Bravais lattice, a qualitative ideas of point and space group; crystal planes and Miller indices, reciprocal lattice.

X-ray diffraction by crystal, Bragg's law, a simple description of rotating crystal method and powder pattern methods. Analysis of powder pattern of simple cubic systems.

Unit – III: Mass spectroscopy & Chromatography

Mass spectroscopy: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making

liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

Chromatography: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Basic Instrumentation Principles of Gas Chromatography Mass Spectroscopy (GCMS) and Liquid Chromatography Mass Spectroscopy (LCMS) and Applications.

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.
- L. V. Azaroff Introduction to Solid, Tata Mcgraw Hill
- Cullity, B. D., *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, **1959**.

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
CHE VOT 405.1	Learn about the basic fundamental laws of UV, FT-IR spectroscopies and selection rules.	2					1	2		1		2
CHE VOT 405.2	Learn the basic introduction and applications of X-Ray Diffraction.	2		3			1	2	2	1		2
CHE VOT 405.3	Basic introduction and applications of Mass spectroscopy & Chromatography.	2	2	2	3	1			2			1

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

PAPER CODE: CHE VOT/I 406: Hands Training of Instruments

Full Mark 50 (30 + 20)

Course Objectives: The learners are Able to: Learn about the basic concepts and hands and training application XRD, UV, Fluorescence spectroscopy, GCMS and LCMS.

D. SYLLABUS

1. Determination of λ_{max} of different standard solutions by UV-vis spectroscopy measurement.
2. Determination of λ_{max} by excitation of a particular wavelength of different standard solutions by fluorescence spectroscopy measurement.
3. Data collection, graph plot and analysis of known/unknown samples by powder X-ray diffraction.
4. Sample analysis of different organic compounds by GCMS and LCMS.

COURSES OF STUDIES

FOR UNDER 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: CHE DMT 101/CHE IDMT 103: Atomic Structure, Chemical Bonding, Fundamentals, Stereochemistry and Hydrocarbons

SYLLABUS

Part-A

Inorganic Chemistry– I: Atomic Structure & Chemical Bonding,

Unit –I: Atomic Structure

Bohr's theory, its limitations and atomic spectrum of hydrogen atom. Wave mechanics: de Broglie equation, Heisenberg's Uncertainty Principle and its significance, Schrödinger's wave equation, significance of ψ and ψ^2. Quantum numbers and their significance. Types of wave functions. Radial and angular wave functions for hydrogen atom. Radial and angular distribution curves. Shapes of *s*, *p*, *d* and *f* orbitals. Contour boundary and probability diagrams.

Pauli's Exclusion Principle, Hund's rule of maximum multiplicity, Aufbau's principle and its limitations, Variation of orbital energy with atomic number.

Unit – II: Chemical Bonding

(i) *Ionic bond:* General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Landé equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Born-Haber cycle and its application, Solvation energy

(ii) *Covalent bond:* Lewis structure, Valence Bond theory (Heitler-London approach). Formal charge, Valence shell electron pair repulsion theory (VSEPR), shapes of simple molecules and ions containing lone pairs and bond pairs of electrons, multiple bonding (σ and π bond approach) and bond lengths. Energetics of hybridization. Bent's rule, Resonance and resonance energy, Molecular orbital theory. Molecular orbital diagrams of diatomic and simple polyatomic molecules N_2, O_2, C_2, B_2, F_2, CO, NO, and their ions; HCl, BeF_2, CO_2, (idea of s-p mixing and orbital interaction to be given).

Covalent character in ionic compounds, polarizing power and polarizability. Fajan's rules and consequences of polarization.

Ionic character in covalent compounds: Bond moment and dipole moment. Percentage ionic character from dipole moment and electronegativity difference.

(iii) *Metallic Bond & Weak Chemical Forces:* Qualitative idea of valence bond and band theories. Semiconductors and insulators, defects in solids, van der Waals forces, ion-dipole forces, dipole-dipole interactions, induced dipole interactions, Repulsive forces, Hydrogen bonding, effects of chemical force, melting and boiling points, solubility energetics of dissolution process.

Unit – III: Redox

Redox equations, Standard electrode potentials, redox potentials and formal potentials, Nernst equation, redox potentials to explore the feasibility of reaction and calculation of values of equilibrium constant,

redox potential as a function of pH, precipitation and complex formation, redox titrations and redox indicators, Frost and Latimer diagrams of redox potentials. Reversible and irreversible cells. Concept of EMF of a cell. Measurement of EMF of a cell.

Part B

Organic Chemistry – I : Fundamentals, Stereochemistry and Hydrocarbons

Unit I: Structure, Reactivity and Mechanism

Atomic orbitals, Hybridization, Bonding in Carbon Compounds, The breaking and forming of bonds, Factors Influencing Electron availability, Steric factors, Reagents types and Reaction types. Kinetics of reaction and Investigation of Reaction Mechanism.

Unit II: The strength of acids and bases

Definition, Various types of acids and bases (Lewis acid, Bronsted acids). The origin of acidity and basicity in organic compounds, The strength of acids and bases with comparative study.

Unit III: Basics of Stereochemistry

Chirality, Configuration and conformation, Geometrical isomerism, Optical isomerism, Enantiomers, Diastereomers, projection formulae, D-L and R-S nomenclature (CIP rules), Erythro and threo nomenclature. dl- and meso compounds, Atropisomerism, Stereospecific and stereoselective reactions, Conformations vs reactivity of cycloalkanes.

Unit IV: Hydrocarbons and Their Functional Groups

Alkenes and alkynes: Synthesis through elimination, electrophilic addition reactions: addition of halogens, hydrogen halides, water, oxymercuration-demercuration, addition of borane; hydrogenation, oxidation, ozonolysis.

Alkyne synthesis, addition of halogen, hydrogen halide, water, boranes, hydrogenation, acetylide ion

Aromaticity, antiaromaticity, Electrophilic aromatic substitution: nitration, halogenation, sulfonation, Friedel-Crafts alkylation and acylation reactions, reactions of substituted benzene: electronic effect of substituents, important reactions of phenols, thiols, aromatic amino compounds and naphthalene. Nucleophilic aromatic substitution: substitution of hydrogen, substitution of atoms other than hydrogen, substitution via aryne intermediates.

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

CHE DMP 107/CHE IDMP 108: Inorganic Chemistry Practical – I

SYLLABUS

(A) Titrimetric Analysis

(i) Calibration and use of apparatus
(ii) Preparation of solutions of different Molarity/Normality of titrants

(B) Acid-Base Titrations

(i) Estimation of carbonate and hydroxide present together in mixture.
(ii) Estimation of carbonate and bicarbonate present together in a mixture.
(iii) Estimation of free alkali present in different soaps/detergents

(C) Oxidation-Reduction Titrimetry

(i) Estimation of Fe(II) and oxalic acid using standardized $KMnO_4$ solution.
(ii) Estimation of oxalic acid and sodium oxalate in a given mixture.
(iii) Estimation of Fe(II) with $K_2Cr_2O_7$ using internal (diphenylamine, anthranilic acid) and external indicator.

OR

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

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

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

SECOND SEMESTER

PAPER CODE: CHE DMT 201/CHE IDMT 203: Thermodynamics – I, Ionic Equilibria, Conductance, Periodicity, Acid-Bases & Radioactivity

SYLLABUS

Part- A

Physical Chemistry – I: Thermodynamics – I, Ionic Equilibria & Conductance

Unit – I: Thermodynamics – I

Introduction of different terms and processes in thermodynamics: [systems (isolated, closed, open) and surrounding, macroscopic properties (extensive and intensive), kinds of processes], state and path functions and their differentials. Zeroth law of thermodynamics.

First Law: concept of heat, *q*, work, *w*, internal energy, *U*, sign convention for heat and work; statement of first law; enthalpy, *H*; heat capacities (C_v, C_p) and relation between them for ideal gases. Reversible and irreversible processes, maximum work; calculations of *q*, *w*, *U* and *H* for reversible, irreversible and free expansion of gases (ideal and van der Waals) under isothermal and adiabatic conditions. Ideal gas law for adiabatic reversible expansion, comparison of adiabatic and isothermal reversible expansion. Joule-Thomson effect, Joule-Thomson coefficient in ideal and real (van der Waals) gases, inversion temperature.

Thermochemistry: Standard state, standard enthalpy of formation, Hess's Laws of constant heat summation and its application. Change in internal energy (ΔU) and enthalpy (ΔH) of chemical reactions, relation between ΔU and ΔH, variation of heat of reaction with temperature (Kirchhoff's equation). Enthalpy of neutralization. Bond Energy – Bond dissociation energy and its calculation from thermo-chemical data. Adiabatic flame temperature and explosion temperature.

Unit – II: Ionic Equilibria

Arrhenius theory of electrolytic dissociation: strong, moderate, and weak electrolytes, degree of ionization, factors affecting degree of ionization, ionization constant and ionic product of water. Ionization of weak acids and bases, pH scale, common ion effect; dissociation constants of mono-, di-and triprotic acids (exact treatment).

Salt hydrolysis – calculation of hydrolysis constant, degree of hydrolysis and pH for different salts. Buffer solutions, derivation of Henderson-Hasselbalch equation and its applications; buffer capacity, buffer range, buffer action and applications of buffers in analytical chemistry and biochemical processes in the human body.

Multistage equilibria in polyelectrolyte systems; hydrolysis and hydrolysis constants.

Theory of acid–base indicators; selection of indicators and their limitations.

Solubility and solubility product of sparingly soluble salts – applications of solubility product principle.

Qualitative treatment of acid – base titration curves (calculation of pH at various stages).

Unit – III: Conductance

Conductivity, equivalent and molar conductivity and their variation with dilution for weak and strong electrolytes (Kohlrausch square root law). Molar conductivity at infinite dilution. Kohlrausch law of independent migration of ions. Debye-Hückel-Onsager equation, Wien effect, Debye-Falkenhagen effect, Walden's rules.

Ionic velocities, mobilities and their determinations, transference numbers and their relation to ionic mobilities, determination of transference numbers using Hittorf and Moving Boundary methods. Applications of conductance measurement: (i) degree of dissociation of weak electrolytes, (ii) ionic

product of water (iii) solubility and solubility product of sparingly soluble salts, (iv) conductometric titrations, and (v) hydrolysis constants of salts.

Quantitative aspects of Faraday's laws of electrolysis, rules of oxidation/reduction of ions based on half-cell potentials, applications of electrolysis in metallurgy and industry.

Part - B

Inorganic Chemistry – II: Periodicity, Acid-Bases & Radioactivity

Unit – I: Periodicity

Periodic table and *s*, *p*, *d*, *f* block elements. Detailed discussion of the following properties of the elements, with reference to *s* & *p*-block.

(a) Effective nuclear charge, shielding or screening effect, Slater rules, variation of effective nuclear charge in periodic table, (b) Atomic radii (van der Waals), (c) Ionic and crystal radii, (d) Covalent radii (octahedral and tetrahedral), (e) Ionization enthalpy, Successive ionization enthalpies and factors affecting ionization energy. Applications of ionization enthalpy. (f) Electron gain enthalpy, trends of electron gain enthalpy. (g) Electronegativity, Pauling's/ Mulliken's/ Alfred-Rochow scales / and Mulliken-Jaffé's electronegativity scales. Variation of electronegativity with bond order, partial charge, hybridization, group electronegativity. Sanderson's electron density ratio.

Unit – II: Acid & Bases

Arrhenius, Brönsted-Lowry, Lux-Flood, Lewis acid-base concepts and reactions, solvated proton, relative strength of acids, types of acid-base reactions, levelling solvents, Factors affecting strengths of Lewis acids and bases, Classification of acids and bases as hard and soft, Pearsons HSAB concept, acid-base strength and hardness and softness, symbiosis, application of HSAB theory.

Non-aqueous solvents

Physical properties of a solvent, types of solvents and their general characteristics, reactions in non-aqueous solvents with reference to liquid NH_3, liquid SO_2 and liquid HF.

Unit – III: Radioactivity

Radioactive decay, half life and average life of radio elements, units of radioactivity, natural radioactive disintegration series, Instrumental analysis of radioactive elements, radioactive equilibrium, group displacement law, isotope, isotone, isobars and nuclear isomerism. Application of isotope in medicine, agriculture, reaction mechanism (isotope as tracer), age of minerals, age of earth, radio carbon dating, nuclear particles, nuclear forces: meson exchange theory.

Nuclear models (elementary idea), nuclear stability, nuclear binding energy, nuclear reactions, magic numbers, mass defect, proton-neutron ratio, packing fraction, Artificial radioactivity, transmutation of elements, fission, fusion and spallation reaction. Nuclear energy, hazards of nuclear radiations and safety measures.

PAPER CODE: CHE DMP 207/CHE IDMP 208: Physical Chemistry Practical – I

A. SYLLABUS

Thermochemistry:

- Determination of heat capacity of a calorimeter for different volumes using change of enthalpy data of a known system (method of back calculation of heat capacity of calorimeter from known enthalpy of solution or enthalpy of neutralization).
- Determination of heat capacity of the calorimeter and enthalpy of neutralization of hydrochloric acid with sodium hydroxide.
- Calculation of the enthalpy of ionization of ethanoic acid.
- Determination of heat capacity of the calorimeter and integral enthalpy (endothermic and exothermic) solution of salts.
- Determination of basicity/proticity of a poly-protic acid by the thermo-chemical method in terms of the changes of temperatures observed in the graph of temperature versus time for different additions of a base. Also calculate the enthalpy of neutralization of the first step.
- Determination of enthalpy of hydration of copper sulfate.
- Study of the solubility of benzoic acid in water and determination of ΔH.

Surface tension measurements:

- Determine the surface tension by (i) drop number.
- Study the variation of surface tension of detergent solutions with concentration.
- Surface tension composition curve for a binary liquid mixture.

Viscosity measurement using Ostwald's viscometer:

- Determination of viscosity of aqueous solutions of (i) polymer (ii) ethanol and (iii) sugar at room temperature.
- Study the variation of viscosity of sucrose solution with the concentration of solute.
- Viscosity composition curve for a binary liquid mixture.

pH metry

- Study the effect on pH of addition of HCl/NaOH to solutions of acetic acid, sodium acetate and their mixtures.
- Preparation of buffer solutions of different pH by
  - **(a)** Sodium acetate-acetic acid
  - **(b)** Ammonium chloride-ammonium hydroxide
- pH metric titration of (i) strong acid *versus* strong base, (ii) weak acid *versus* strong base.
- Determination of dissociation constant of a weak acid.
- To study the dissociation constant of amino acid (glycine) and hence the isoelectric point of the acid.

Conductometry:

- Determination of cell constant.
- Determination of equivalent conductance, degree of dissociation and dissociation constant of a weak acid.
- Perform the following conductometric titrations:
  - **(a)** Strong acid *versus* strong base
  - **(b)** Weak acid *versus* strong base
  - **(c)** Dibasic acid *versus* strong base

Any other experiment carried out in the class if permit.

SEMESTER – III

PAPER CODE: CHE DMT 301/ CHE IDMT 303

Substitution, Elimination Reactions, Carbonyl Chemistry, Thermodynamics-II, Electrochemistry, and Chemical Kinetics.

SYLLABUS

Part – A

Organic Chemistry – II: Substitution, Elimination Reactions, and Carbonyl Chemistry

Unit – I: Nucleophilic Substitution Reactions at a Saturated Carbon atom (sp^3 Carbon)

Types of Substitution reactions (S_N1, S_N2, S_Ni), neighboring group participation (NGP), factors affecting various SN-type reactions, Competition between S_N1 and S_N2 reactions, Substitution reactions of alcohols, alkyl halides, reactions with epoxides (regioselectivity on acid and base medium).

Unit – II: Elimination Reaction

1,2-(β-) Elimination, E1 Mechanism, E1cb Mechanism, E2 Mechanism, Elimination vs Substitution, Factors affecting Elimination Reactions, 1,1-(α-)Elimination, Pyrolytic Syn Elimination

Unit – III: Nucleophilic addition to C=O (Carbonyl Chemistry)

Addition Reactions at sp^2 Carbons: Addition of Carbon, Hydrogen, oxygen, sulfur and Nitrogen nucleophiles to Carbonyl Compounds, Wittig reaction, Cannizzaro's reaction, α,β-unsaturated carbonyl compounds-preparation and properties, Michael addition, 1,2 Vs 1,4- addition reaction.

Acidity of α-hydrogen: Keto-enol tautomerism, alkylation, acylation, halogenation, Aldol condensation, Robinson annulation, Perkin's reaction, Claisen condensation, Dieckmann condensation Reaction, Stobbe Condensation Reaction, Bamford-Steven, Shapiro reaction, base-catalyzed halogenations reaction of ketones (haloform reactions,), active methylene compounds and their reactions, Malonic ester (DEM), acetoacetic ester (EAA).

Carboxylic acid and its derivatives (esters, anhydrides, acid halides, amides): Relative Reactivities, Nucleophilic acyl substitution reactions, Synthesis and reactions.

Part – B

Physical Chemistry - II: Thermodynamics-II, Electrochemistry, and Chemical Kinetics

Unit – I: Thermodynamics – II

Second Law: Limitation of first Law, spontaneous processes and different statement of second law of thermodynamics, Carnot cycle and its efficiency, Carnot theorem; thermodynamic scale of temperature.

Concept of Entropy: Entropy changes in reversible and irreversible processes and of universe, physical concept of entropy (molecular and statistical interpretation of entropy), Calusius inequality; entropy as a function of *V* & *T*, and *P* & *T*; entropy changes of an ideal gas in different processes, entropy change in mixing of gases.

Free Energy Functions: Free energy and its concept, Gibbs (*G*) and Helmholtz (*A*) free energies as thermodynamic quantities and their relationship; variation of free energy with temperature and pressure. Maxwell's relations, thermodynamic equation of state; criteria for reversible and irreversible processes (spontaneity); Gibbs-Helmholtz equations, its application of the determination of ΔG, ΔH, ΔS of a reversible cell reaction.

Third Law: Variation of entropy with temperature (Nernst heat theorem), statement of third law, the concept of residual entropy. Applications of third law for determination of absolute entropies of liquid and gases.

Unit – II: Electrochemistry

Chemical cells, reversible and irreversible cells with examples. Electromotive force of a cell and its measurement, Nernst equation; Single electrode potential, its measurement and sign convention. Standard electrode (reduction) potential and its application to different kinds of half-cells. Application of EMF measurements in determining (i) free energy, enthalpy and entropy of a cell reaction, (ii) equilibrium constants, and (iii) pH values, using hydrogen, quinone-hydroquinone, glass and SbO/Sb_2O_3 electrodes (iv) qualitative discussion of potentiometric titrations (acid-base, redox, precipitation). Concentration cells with and without transference, liquid junction potential and its elimination; determination of activity coefficients and transference numbers. Fuel cell (Hydrogen-Oxygen), Commercial Cell (Primary & Secondary cell), dry cell, acid-alkali storage cell & introduction of lithium ion cells.

Unit – III: Chemical Kinetics

The concept of reaction rate, order and molecularity of a reaction, rate laws in terms of the advancement of a reaction, differential and integrated form of rate expressions up to second order reactions, experimental methods of the determination of rate laws; half-life of a reaction.

Temperature dependence of reaction rates; Arrhenius equation; activation energy. Collision theory of reaction rates, qualitative treatment of the theory of absolute reaction rates.

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PAPER CODE: CHE DMP 307/CHE IDMP 308: Organic Chemistry Practical – I

Full Mark 50

A. SYLLABUS

1. Determination of the melting points of known and unknown organic compounds (Kjeldahl method and electrically heated melting point apparatus)
2. Chromatography

a. Separation of a mixture of two amino acids by ascending and horizontal paper chromatography
b. Separation of a mixture of two sugars by ascending paper chromatography
c. Separation of a mixture of o-and p-nitrophenol or o-and p-aminophenol by thin layer chromatography (TLC)

Qualitative Analysis

3. a. Detection of special elements N, S and halogen (X = Cl, Br and I)
b. Detection of non-nitrogenous Functional groups (alcohols, phenols, carbonyl and carboxylic acid and ester functional groups)
c. Detection of nitrogenous Functional groups (primary nitro, amine and amide functional groups)

4. Identification of functional groups present in a unknown organic sample (Qualitative analysis of unknown organic compounds containing simple functional groups such as alcohols, carboxylic acids, phenols, carbonyl compounds, nitro, amine and amide groups)

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SEMESTER – IV

PAPER CODE: CHE DMT 401/CHE IDMT 403: Chemistry of -s, -p, -d and -f Block elements, Rearrangement and Reagents in Organic Chemistry

SYLLABUS

Part – A

Inorganic Chemistry-III: Chemistry of *-s, -p, -d and -f* Block elements

Unit – I: *-s & p-Block Elements:*

s-Block Elements: General characteristic properties, complexes of alkali metals, comparative study of hydrides, oxides, hydroxides, halides, carbonates and bicarbonates of group I and II, Diagonal relationship, Allotropy and catenation, Biological role of alkali and alkaline earth metals.

p-Block Elements: General characteristic properties, comparative study (including diagonal relationship and inert pair effect) of groups 13-17 (B, C, N, O, F) elements and group trends of compounds like hydrides, oxides, halides, and oxy acids.
Study of the following compounds with emphasis on structure, bonding, preparation, properties and uses (Inorganic Polymers): Boric acid and borates, boron nitrides, borohydrides (diborane) carboranes and graphitic compounds, fullerenes, silanes, Oxides and oxoacids of nitrogen, Phosphorus and chlorine. Peroxo acids of sulphur, halogens, interhalogen compounds, polyhalide ions, and pseudohalogens.

Unit – II: d-Block and Inert Group 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

Noble Gases: Occurrence and uses, rationalization of inertness of noble gases, Clathrates; preparation and properties of XeF_2, XeF_4 and XeF_6; Nature of bonding in noble gas compounds (Valence bond treatment and MO treatment for XeF_2). Molecular shapes of noble gas compounds (VSEPR theory).

Unit – III: f-Block Elements:

Chemistry of Lanthanides & Actinides: **E**lectronic configuration, oxidation states, colour, spectral and magnetic properties, lanthanide contraction, separation of lanthanides and actinides (ion-exchange method only), important lanthanide compounds, similarities the later actinides and lanthanides elements.

Part – B

Organic Chemistry – III : Rearrangement and Reagents in Organic Chemistry

Unit – I: Rearrangement Reactions

Reactive intermediates and name reactions: Generation, structure, stability and reactions involving the intermediates: Carbocation (Pinacol-Pinacolone Rearrangement, Wagner-Meerwein Rearrangement, Demjanov reaction, Favorski Rearrangement, Fries Rearrangement, Benzil-Benzilic Acid

Rearrangement), carbanion (Alkylation, Aldol condensation, Robinson annulation, Claisen condensation, Dieckmann condensation Reaction, Perkin Reaction, Stobbe Condensation Reaction, Bamford-Steven, Shapiro reaction), Free radicals (Allylic halogenations, acyloin condensation, McMurry coupling, Hunsdiecker reaction, Bouveault-Blanc reduction), carbenes (Wolff Rearrangement, Reimer-Tiemann), nitrenes (Hofmann, Beckmann, Curtius, Schmidt, Lossen Rearrangement), arynes, ylides (Wittig Reaction).

Unit – II: Oxidizing reagents

Chromium reagents, manganese reagents, Ruthenium tetroxide, TPAP, Lead tetraacetate, Osmium tetroxide, Hypervalent Iodine reagents [Dess-Martin periodinane (DMP), o-iodoxybenzoicacid (IBX)], Cerric ammonium nitrate, DDQ, Selenium dioxide, DMSO based oxidizing reagents, Aluminiumalkoxides (Oppenauer Oxidation), peroxyacids (epoxidation and Baeyer-Villiger oxidation of ketones)

Unit – III: Reducing reagents

Heterogeneous Catalytic hydrogenation, Homogeneous Catalytic hydrogenation (Wilkinson's Catalyst), Dissolving metal reduction (Clemmesen Reduction Reaction, Birch Reduction) Reduction with hydride-transfer reagents (Aluminiumalkoxides, Lithium aluminium hydride, sodium borohydride, DIBAL-H, Tinhydrides, Silanes, diimide, Borane and derivatives.

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PAPER CODE: CHE DMP 407/CHE IDMP 408: Physical Chemistry Practical – II

A. SYLLABUS

Chemical Equilibrium:

- Equilibrium constant of methyl acetate hydrolysis reaction.
- Determination of critical solution temperature and composition of the phenol-water system and to study the effect of impurities on it.
- Phase equilibria: Construction of the phase diagram using cooling curves or ignition tube method:
  (a) simple eutectic and **(b)** congruently melting systems
- Distribution of acetic/ benzoic acid between water and cyclohexane.
- Study the equilibrium of at least one of the following reactions by the distribution method:

(a) $I_2(aq) + I^-(aq) \rightleftharpoons I_3^-(aq)$ and **(b)** $Cu^{2+}(aq) + nNH_3(aq) \rightleftharpoons [Cu(NH_3)_n]^{2+}$

Chemical Kinetics:

- Study the kinetics of the following reactions.

(a) Initial rate method: Iodide-persulphate reaction.
(b) Order of reaction of I_2 – acetone – H^+ ion.
(c) Integrated rate method:
(d) Acid hydrolysis of methyl acetate with hydrochloric acid
(e) Saponification of ethyl acetate.
(f) Compare the strengths of HCl and H_2SO_4 by studying kinetics of hydrolysis of methyl acetate.

Potentiometry:

- Perform the following potentiometric titrations:

(a) Strong acid *versus* strong base
(b) Weak acid *versus* strong base
(c) Dibasic acid *versus* strong base

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SEMESTER – V

PAPER CODE: CHE DMT 501/CHE IDMT 503: Photochemistry, Catalysis, Quantum Chemistry & Spectroscopy

A. SYLLABUS

Unit – I: Photochemistry

Characteristics of electromagnetic radiation and interaction of radiation with matter, difference between thermal and photochemical processes. Laws of photochemistry: Grothus-Drapper law, Stark-Einstein law, Jablonski diagram depicting various processes occurring in the excited state, qualitative description of fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing). Lambert-Beer's law and its limitation, physical significance of absorption coefficient; quantum efficiency, reasons for low and high quantum efficiency. Kinetics of photochemical reactions ($H_2 + Br_2 = HBr$ and $2HI = H_2 + I_2$), photostationary state. Chemical actinometers (ferri-oxalate, uranyl oxalate, MGL [malachite green leucocyanide)] and Reinecke's salt); chemiluminescence, role of photochemical reactions in biological process.

Unit – II Catalysis

Type of catalysts, specificity and selectivity, mechanism of catalyzed reaction at solid surface; effect of temperature on surface reaction, promoters and poisons.

***Heterogeneous Catalysis* (*Surface Reactions*):** Physical adsorption, chemisorptions, nature of adsorbed state, adsorption isotherm; Langmuir and Freundlich adsorption isotherms. Multi-layer adsorption-BET equation (no derivation) and its application to surface area measurement.

Kinetics Homogeneous Catalysis: Nature of surface, concept of active centres. Kinetics of enzymatic reactions: Michaelis-Menten equation, Lineweaver-Burk and Eadie plot, effect of temperature and pH.

Unit – III: Complex reactions

Kinetics of complex reactions (integrated rate expressions up to first order only): (i) opposing reactions (ii) parallel reactions and (iii) consecutive reactions and their differential rate equations (steady-state approximation in reaction mechanisms) (iv) chain reactions (v) uni molecular gas reaction (Lindemann mechanism)

Unit – IV Quantum Chemistry and Spectroscopy – I

Spectroscopy and its importance in chemistry. Wave-particle duality. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. Types of spectroscopy. Difference between atomic and molecular spectra. Born-Oppenheimer approximation: Separation of molecular energies into translational, rotational, vibrational and electronic components.
Postulates of quantum mechanics, quantum mechanical operators.
Free particle. Particle in a 1-D box (complete solution), quantization, normalization of wave functions, concept of zero-point energy.

Unit – V Quantum Chemistry and Spectroscopy – II

Rotational Motion: Schrödinger equation of a rigid rotator and brief discussion of its results (solution not required). Quantization of rotational energy levels.
Microwave (pure rotational) spectra of diatomic molecules. Selection rules. Structural information derived from rotational spectroscopy.

Vibrational Motion: Schrödinger equation of a linear harmonic oscillator and brief discussion of its results (solution not required). Quantization of vibrational energy levels. Selection rules, IR spectra of diatomic molecules. Structural information derived from vibrational spectra. Vibrations of polyatomic molecules. Group frequencies. Effect of hydrogen bonding (inter- and intramolecular) and substitution on vibrational frequencies.

Electronic Spectroscopy: Electronic excited states. Free Electron model and its application to electronic spectra of polyenes. Color and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

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PAPER CODE: CHE DMP 507/CHE IDMP 508: Physical Chemistry Practical – III

A. SYLLABUS

Catalysis:

- Kinetics of enzymation reaction (starch-amylase system).
- Kinetics of catalytic decomposition of H_2O_2

Surface Chemistry:

- Verify the Freundlich and Langmuir isotherms for adsorption of acetic acid on activated charcoal.

Photochemistry:

- Photochemical reduction of ferric oxalate in cyanotype blue printing.

UV/Visible spectroscopy:

- Study the 200-500 nm absorbance spectra of $KMnO_4$ and $K_2Cr_2O_7$ (in 0.1 M H_2SO_4) and determine the λ_{max} values. Calculate the energies of the two transitions in different units (J molecule^{-1}, kJ mol^{-1}, cm^{-1}, eV).
- Study the pH-dependence of the UV-Vis spectrum (200-500 nm) of $K_2Cr_2O_7$.
- Record the 200-350 nm UV spectra of the given compounds (acetone, acetaldehyde, 2-propanol, acetic acid) in water. Comment on the effect of structure on the UV spectra of organic compounds.

Colorimetry:

- Verify Lambert-Beer's law and determine the concentration of $CuSO_4$/$KMnO_4$/$K_2Cr_2O_7$ in a solution of unknown concentration.
- Determine the concentrations of $KMnO_4$ and $K_2Cr_2O_7$ in a mixture.
- Study the kinetics of iodination of propanone in acidic medium.
- Determine the amount of iron present in a sample using 1,10-phenathroline.
- Determine the dissociation constant of an indicator (phenolphthalein).
- Study the kinetics of interaction of crystal violet/phenolphthalein with sodium hydroxide.
- Analysis of the given vibration-rotation spectrum of HCl(g)

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PAPER CODE: CHE DMT/I 505: Chemistry Research Orientation

A. SYLLABUS

Unit – I: Why Students Interested on Chemistry Research?

Research Overview, Importance of Chemistry Research, Types of application in today's chemistry

Unit – II: Research Outline

Before start the research area/topic search outline of the research related topics with the help of Journals, Reviews, monographs, dictionaries, text-books etc.

Digital Sources: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, UGC infonet, E-books, Internet discussion groups and communities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider.

Outline of Journals: Elsevier, ACS, RSC, Springer, Wiley, MDPI etc.

Article format: Title, Authors, Affiliation, Abstract, Keywords, Introduction, Experimental Section, Characterization, Results & Discussion, Conclusion, Acknowledgements & References

Unit – III: Chemical Safety and Ethical Handling of Chemicals:

Safe working procedure and protective environment, protective apparel, emergency procedure and first aid, laboratory ventilation. Safe storage and use of hazardous chemicals, procedure for working with substances that pose hazards, flammable or explosive hazards, procedures for working with gases at pressures above or below atmospheric – safe storage and disposal of waste chemicals, recovery, recycling and reuse of laboratory chemicals, procedure for laboratory disposal of explosives, identification, verification and segregation of laboratory waste, disposal of chemicals in the sanitary sewer system, incineration and transportation of hazardous chemicals.

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PAPER CODE: CHE DMP/I 509: Organic Chemistry Practical – II

A. SYLLABUS

Quantitative analysis

A. Organic preparations (Any six organic preparation from the following suggested topics have to be completed)

a. Acetylation of one of the following compounds: amines (aniline, o-, m-, p-toluidines and o-, m-, p-anisidine) and phenols (β-naphthol, vanillin, salicylic acid) by any one method:
   1. Using conventional method
   2. Using Green Method

b. Benzolyation of one of the following amines (aniline, o-, m-, p- toluidines and o-, m-, p-anisidine) and one of the following phenols (β-naphthol, resorcinol, p-cresol) by Schotten-Baumann reaction.

c. Oxidation of ethanol/ isopropanol (Iodoform reaction).

d. Bromination of any one of the following:
   1. Acetanilide by conventional methods
   2. Acetanilide using green approach (Bromate-bromide method)

e. Nitration of any one of the following:
   1. Acetanilide/nitrobenzene by conventional method
   2. Salicylic acid by green approach (using ceric ammonium nitrate)

f. Reduction of p-nitrobenzaldehyde by sodium borohydride.

g. Hydrolysis of amides and esters.

h. Aldol condensation: Preparation of chalcone substrate.

i. Azo compound preparation (Methyl orange)

j. Racemic BINOL preparation from β-naphthol using FeCl3.

The above derivatives should be prepared using 0.5-1g of the organic compound. The solid samples must be collected and may be used for recrystallization, melting point and TLC.

B. Estimation (Any Three estimations from the following experiments have to be done)

a. Estimation of glycine by Sorenson's formalin method.
b. Study of the titration curve of glycine.
c. Saponification value of an oil or a fat.
d. Determination of Iodine number of an oil/ fat.
e. Isolation and characterization of DNA from onion/ cauliflower/peas.

SEMESTER – VI

PAPER CODE: CHE DMT 601/CHE IDMT 604: Coordination & Organometallics Chemistry

A. SYLLABUS

Unit – I: Coordination Chemistry

Werner's theory, IUPAC nomenclature of coordination compounds, Types of isomerism in coordination compounds: Constitutional, geometrical and optical isomerism in respect of coordination numbers 4 and 6, Determination of configuration of cis-, trans-isomers by chemical methods.
Valence bond theory (inner and outer orbital complexes), electroneutrality principle and back bonding. Crystal field theory, measurement of 10 Dq (o), CFSE in weak and strong fields, pairing energies, factors affecting the magnitude of 10 Dq (o, t). Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, square planar geometry. Qualitative aspect of Ligand field and MO Theory, Chelate effect, polynuclear complexes.

Unit – I: Electronic Spectra of Transition Metal Complex

Introduction to electronic spectra of transition metal complexes, Orgel diagrams for $3d^1$-$3d^9$ ions, selection rules, d-d/charge transfer spectra, Colour, spectrochemical series, Nephelauxetic effect, trans effect, (example and applications) labile and inert complexes. Difference between the first, second and third transition series.

Chemistry of Ti, V, Cr Mn, Fe and Co in various oxidation states (excluding their metallurgy)

Unit – III: Magnetic Properties of Transition Metal

Types of magnetic behaviour, methods of determining magnetic susceptibility, spin only formula, L-S coupling, Orbital contribution to magnetic moments, quenching of magnetic moment, super-exchange, antiferromagnetic interaction (elementary idea with examples only), application of spin only values of magnetic moments to determine valency and stereochemistry of coordination compounds (based on VBT and CFT)

Unit – IV: Bioinorganic Chemistry

Elements of life: essential major, trace and ultratrace elements. Basic chemical reactions in the biological systems and the role of metal ions (specially Na^+, K^+, Mg^{+2}, Ca^{+2}, $Fe^{3+/2+}$, Cu^{+2}, and Zn^{+2}). Haemoglobin, myoglobin, chlorophyll, cytochromes, ferredoxins and carbonic anhydrase-their structural features and functions in living system.
Toxic metal ions and their effects, lead, mercury, cadmium and arsenic poisoning, organo-mercury compounds; Use of chelating agents in medicine: Wilson diseases, detoxification of metal ions – chelation therapy (simple idea with some examples of chelating drugs). Pt and Au complexes as drugs (examples only), metal dependent diseases.

Unit – V: Organometallic Chemistry

Definition and classification of organometallic compounds on the basis of bond type. Concept of hapticity of organic ligands.

Metal carbonyls: 18 electron rule, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. General methods of preparation (direct combination, reductive carbonylation, thermal and photochemical decomposition), Structures of mono and binuclear carbonyls of 3d series.

Zeise's salt: Preparation and structure, evidences of synergic effect and comparison of synergic effect with that in carbonyls, Metal Alkyls: Important structural features of different allyl compounds. Grignard reagent and their structures, Schlenk equilibrium.

Ferrocene: Preparation and reactions (acetylation, alkylation, metallation, Mannich Condensation). Structure and aromaticity. Comparison of aromaticity and reactivity with that of benzene.

Catalysts: Study of the following industrial processes and their reactions & mechanism: Alkene hydrogenation (Wilkinsons Catalyst), Hydroformylation (Co salts), Wacker Process, Synthetic gasoline (Fischer Tropsch reaction), Synthesis gas by metal carbonyl complexes.

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PAPER CODE: CHE DMP 607/CHE IDMP 608: Inorganic Chemistry Practical – III

A. SYLLABUS

(A) Qualitative Estimation of unknown salts

Qualitative semimicro analysis of mixtures containing 2 anions and 2 cations. Emphasis should be given to the understanding of the chemistry of different reactions. The following radicals are suggested:

CO_3^{2-}, NO_2^-, S^{2-}, SO_3^{2-}, $S_2O_3^{2-}$, CH_3COO^-, F^-, Cl^-, Br^-, I^-, NO_3^-, BO_3^{3-}, $C_2O_4^{2-}$, PO_4^{3-}, NH_4^+, K^+, Pb^{2+}, Cu^{2+}, Cd^{2+}, Bi^{3+}, Sn^{2+}, Sb^{3+}, Fe^{3+}, Al^{3+}, Cr^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ba^{2+}, Sr^{2+}, Ca^{2+}, Mg^{2+}

Mixtures should preferably contain one interfering anion, **or** insoluble component ($BaSO_4$, $SrSO_4$, $PbSO_4$, CaF_2 or Al_2O_3) **or** combination of anions e.g. CO_3^{2-} and SO_3^{2-}, NO_2^- and NO_3^-, Cl^- and Br^-, Cl^- and I^-, Br^- and I^-, NO_3^- and Br^-, NO_3^- and I^-.

Spot tests should be done whenever possible

i. Measurement of 10 Dq by spectrophotometric method
ii. Verification of spectrochemical series.
iii. Preparation of acetylacetanato complexes of Cu^{2+}/Fe^{3+}. Find the λ_{max} of the complex.
iv. Synthesis of ammine complexes of Ni(II) and its ligand exchange reactions (e.g. bidentate ligands like acetylacetone, DMG, glycine) by substitution method.

(B) Iodo / Iodimetric Titrations

(i) Estimation of Cu(II) and $K_2Cr_2O_7$ using sodium thiosulphate solution (Iodimetrically).
(ii) Estimation of (i) arsenite and (ii) antimony in tartar-emetic iodimetrically
(iii) Estimation of available chlorine in bleaching powder iodometrically.

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PAPER CODE: CHE DMT 603/CHE DMT 608: Bioorganic Chemistry

SYLLABUS

Unit – I: Carbohydrates

Classification, Monosaccharides, erythro-andthreo-(D/L) sugars, epimers, cyclicstructures of monosaccharides, Haworth projections and other conformational structures, Interconversion of aldoses and ketoses, mutarotation, chain-shortening and lengthening of sugars (Killiani-Fischer synthesis and Ruff degradation), reactions of monosaccharides, reducing and nonreducing sugars, proof of configuration, determinationof ring size, disaccharides (Only structure and properties: maltose, lactose and sucrose) and polysaccharides (Starch, cellulose and glycogen).

Unit – II: Amino acids, Peptides and Proteins

Classification and nomenclature of amino acids, configuration, acid-base properties, isoelectric point, Amino acid synthesis and chemical properties of amino acids. Peptides: peptide bond, sequencing a peptide (N-terminus and C-terminus), Peptide synthesis: solution and solid phase peptide synthesis, biologically importantpeptides (glutathione, oxytocin-important functions). Proteins: Structure of proteins (Primary, Secondary,Tertiary, Quaternary- definition, examples). Forces that stabilize structure of proteins: H-bonds,hydrophobic interaction, electrostatic attraction, Van der Waal's interaction, dipole-dipoleinteraction.

Unit – III: Lipids and Nucleic Acids

Introduction to lipids, Waxes, Triglycerides, Reaction of triglycerides, Phospholipids, Steroids (Cholesterol), Prostaglandin: Structure and functions

Nucleic Acids: Purine and pyrimidine bases of nucleic acids, base pairing via H-bonding, structure of ribonucleic acid (RNA) and deoxyribonucleic acid (DNA), double helix model of DNA and forces responsible for holding it. Chemical synthesis of mono and tri nucleosides. Chemical Properties: Hydrolysis (acid, alkali), enzymatic hydrolysis of DNA. General structure and types of RNA (tRNA, mRNA, rRNA).

Unit – IV: N-containing Functional Groups and Heterocyclic Chemistry N-containing Functional Groups

Introduction to amines, Nomenclature and classification of amines, Properties of amines, Strategies of amine synthesis (via substitution reactions, Reductive amination and Gabriel Phthalimide synthesis), acylation and sulfonylation of amines, Reactions of amines with nitrous acids, Aryl Diazonium salt preparations and reactions (Sandmeyer Reaction).

Heterocyclic Chemistry

Introduction to heterocyclic chemistry, Basics of structures, nomenclature, properties, Synthesis and properties of Furan, Thiophene and Pyrrole, Indole.

Unit – V: Natural Products

Basics of Terpenoids and alkaloids, Isolation and structure elucidation of Terpenoids (Citral, Geraniol, Menthol), alkaloids (Nicotine, atropine).

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SEMESTER – VII

(Honours / PG Course)

PAPER CODE: CHE DMT 701: Transition and Inner Transition Metal Chemistry

A. 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.

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PAPER CODE: CHE DMP 705: Inorganic Practical – III

SYLLABUS

(A) Gravimetric Analysis:

i. Estimation of nickel (II) using Dimethylglyoxime (DMG).
ii. Estimation of copper as CuSCN
iii. Estimation of iron as Fe_2O_3 by precipitating iron as $Fe(OH)_3$.
iv. Estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$ (aluminium oxinate).

(B) Inorganic Preparations:

i. Tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$
ii. *Cis* and *trans* $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)
iii. Tetraamminecarbonatocobalt (III) ion
iv. Potassium tris(oxalate)ferrate(III)

(C) Chromatography Separation of metal ions

- Principles involved in chromatographic separations. Paper chromatographic separation of following metal ions:

i. Ni (II) and Co (II)
ii. Fe (III) and Al (III)

- Chromatographic separation of sugars, amino acids by paper, T.L.C. and Ion exchange.

(D) Estimation of $Fe^{2+/3+}$, Cu^{2+}, Ca^{2+} ions from dichromate/thiosulphate solution.

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PAPER CODE: CHE DMT 702: 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).

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PAPER CODE: CHE DMP 706: ORGANIC CHEMISTRY PRACTICAL - I

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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

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PAPER CODE: CHE DMT 703: Thermodynamics, Catalysis, and Electro- & Surface Chemistry

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.

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PAPER CODE: CHE DMT (I) 704: Research Methodology for Chemistry

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Unit – I: Literature Survey

Print: Sources of information: Primary, secondary, tertiary sources; Journals: Journal abbreviations, abstracts, current titles, reviews, monographs, dictionaries, text-books, current contents, Introduction to Chemical Abstracts and Beilstein, Subject Index, Substance Index, Author Index, Formula Index, and other Indices with examples.

Digital: Web resources, E-journals, Journal access, TOC alerts, Hot articles, Citation index, Impact factor, H-index, E-consortium, UGC infonet, E-books, Internet discussion groups andcommunities, Blogs, Preprint servers, Search engines, Scirus, Google Scholar, ChemIndustry, Wiki- Databases, ChemSpider.

Information Technology and Library Resources: The Internet and World Wide Web. Internet resources for chemistry for finding and citing published information from Science Direct, SciFinder, Scopus.

Unit – II: Methods of Scientific Research and Writing Scientific Papers

Reporting practical and project work. Writing literature surveys and reviews. Organizing a poster display. Giving an oral presentation.

Writing scientific papers – justification for scientific contributions, bibliography, description of methods, conclusions, the need for illustration, style, publications of scientific work. Writing ethics. Avoiding plagiarism.

Unit –III: Research Ethics and Data Analysis

Research Ethics: Copy-writing, Scientific Interpretation, Data manipulation etc. strictly offensive and it should avoid.

Data Analysis

The Investigative Approach: Making and Recording Measurements of experimental products by using sophisticated instruments. Analysis raw data interpret by using different software like Chem-draw, Origin, Excels etc.

Analysis and Presentation of Data: Descriptive statistics. Choosing and using statistical tests. Chemometrics. Analysis of variance (ANOVA), Correlation and regression, Curve fitting, fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals, General polynomial fitting, linearizing transformations, exponential function fit, *r* and its abuse. Basic aspects of multiple linear regression analysis.

Electronics: Basic fundamentals of electronic circuits and their components used in circuits of common instruments like spectrophotometers, typical circuits involving operational amplifiers for electrochemical instruments. Elementary aspects of digital electronics.

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PAPER CODE: CHE DMP/I 707: Chemistry Software Uses for Advanced Research

1. Practical Assignment: Graph plot of XRD, FTIR, UV by apply Origine software,
2. Chemical Structure Draw by using Chem Draw software
3. Seminar
4. Short Project Work

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SEMESTER – VIII

(PG Course)

(Credits: 20; Laboratory & Other Activities: 6 Months; Maximum Marks: 500)

PAPER CODE: CHE D 801: Project & 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. The project work is evaluated by the fulfilment of the following criteria.

	Course Code	Criteria	Credit	Marks
Dissertation/ Project	**CHE D 801**	**D 801: Dissertation/Project**		
	CHE D 801A	• D 801A: Development of project/ Research proposal/Lab Work	**4**	**100**
	CHE D 801B	• D 801B: Pre-Submission presentation/Data collection	**4**	**100**
	CHE D 801C	• D 801C: Report Writing/Write-up/ Dissertation Report	**8**	**200**
	CHE D 801D	• D 801D: Presentation &Viva Voce	**4**	**100**
		Total	**20**	**500**

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SEMESTER – IX

(PG Course)

PAPER CODE: CHE DMT 901: Organometallic Chemistry

A. 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.

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PAPER CODE: CHE DMP 905: Inorganic Chemistry Practical – IV

A. Qualitative Analysis

Semi-micro qualitative analysis of mixture containing six 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. Mixture Separation of Inorganic metal ions:

- 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 by gravimetrically /complexometrically/spectrophotometrically.

C. Preparations of Complex

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, Mercury tetrathiocyanatocobaltate(II), Copper(II) biguanide
4. Mn_{12} Acetate Single Molecule Magnet
5. Preparation of copper glycine complex- cis and transbis- (glycinato) copper (II).
6. 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).
7. $VO(acac)_2$, *cis*-K $[Cr(C_2O_4)_2(H_2O)_2]$, $Na[Cr(NH_3)_2(SCN)_4]$

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PAPER CODE: CHE DMT 902: Principle of Organic Synthesis

A. 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

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PAPER CODE: CHE DMP 906: Organic Chemistry Practical – IV

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.

- Nitrobenzene→aniline→Acetanilide (Nitration and followed by reduction)
- Malonic acid→cinnamicacid→methylcinnamate (Knoevenagel 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→cinnamylalcohol→cinnamylbromide→allyl-aryl ether synthesis (Nucleophilic substitution reaction)

Part B: Characterization of above said synthesized organic compounds using IR, UV and NMR, and mass spectroscopic techniques are to be studied.
Part C: Designing and drawing a reaction scheme and structures using Chemdraw software.

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PAPER CODE: CHE DMT 903: Quantum-, Statistical- Mechanics, Chemical Kinetics

A. 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: Chemical Kinetics

Rate law, method of determining rate laws, General feature of fast reactions, study of fast reaction by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method.

Reactions in Gas Phase: Theories of Reaction Rates- Arrhenius theory, collision theory and transition state theory, potential energy surface, enthalpy, free energy and entropy of activation, correlation of steric factor in collision theory and entropy of activation (Thermodynamic parameter). Uni-molecular reactions: Lindeman-Hinshelwood theory, Rice-Ramsperger-Kasssel (RRK) theory, Rice- Ramsperger-Kassel-Marcus (RRKM) theory.

***Elementary Reactions in Solution*:** Comparison between gas-phase and solution-phase reactions, factor determining reaction rates in solution; ionic reaction [influence of solvent, influence of ionic strength (salt effect)] ; Linear Free Energy Relationships, (LFER), Effect of substituent on reaction rates (Hammet relationships). Kinetic of isotopic effects.

***Dynamic of Molecular Motion*:** probing the transition state, dynamics of barrier-less chemical reaction in solution.

Chain Dynamic: (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reaction), and Oscillatory reaction, autocatalysis (Belousov-Zhabotinsky reaction).

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PAPER CODE: CHE DET 904: Molecular Spectroscopy

A. 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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SEMESTER – X (PG Course)

PAPER CODE: CHE DMT 1001: Bio-Inorganic & Sensor Materials 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: Sensor Materials Chemistry

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.

Different types of Sensing Materials

Metal ion sensing nanomaterials, Dyes sensing nanomaterials, MOFs used as sensing materials, Nanomaterials are used in therapeutic treatment

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PAPER CODE: CHE DMT 1002: 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).

PAPER CODE: CHE DMT 1003: Chemical Bonding, Group Theory, 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: 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.

Unit – 4: Application of Group Theory

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, SF_6, etc.

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: CHE DET 1004A: Introduction to Nanomaterials & Nanotechnology

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); thermal techniques (TG, DTA, DSC), an introduction and basic principles & applications of XPS, FTIR spectrophotometers; UV-VIS principle and application for band gap measurement, magnetic technique-VSM/SQUID.

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.

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PAPER CODE: CHE DET 1004B: Advanced Heterocyclic Chemistry

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.

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PAPER CODE: CHE DMP 1005: Physical Chemistry Practical – IV

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.

(ii) 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.

(iii) (a) Rate of the hydrolysis of sucrose using polarimeter.

(b) Polarizability from refractive index measurement.

(iv) 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.

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

IR and Raman spectroscopy of the solvent mixture.

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CHE DMP 1006A: Nanomaterials Chemistry Practical

SYLLABUS

Nano Materials Chemistry

- Verification of the Beer-Lambert law using gold/silver nanoparticles.
- Preparation and characterization of nanomaretials by wet chemical routes (sol-gel, reverse micelles, hydrothermal, co-precipitation, *etc*.)
- Synthesis and characterization of core-shell nanocomposite (bimetallic and oxides)
- Synthesis and characterization of mixed metal oxide (bimetallic and oxides)
- Metal based nanoparticles are examined by converting *p*-nitrophenol to *p*-aminophenol.
- Determination of the band gap of semiconductor nanomaterials.
- Study of surface enhanced Raman scattering activity of silver nanostructures.
- Study dye degradation of synthesized nanoparticles by UV/Visible light.

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CHE DMP 1006B: Advanced Heterocyclic Chemistry Practical

SYLLABUS

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.

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Minor Paper in Chemistry
(Disciplinary Minor/Inter-disciplinary Minor)

Minor Paper in Chemistry							
Semester	Course Code	Course Name	Marks		Total Marks	Duration (Hrs) of Exam (End Term	Credit
			END TERM	MID TERM			
I	CHE DMI 102 & CHE IDMI 104	States of Matter and Colloidal State	30	20	50	2	2
II	CHE DMI 202 & CHE IDMI 204	Chemistry in Daily Life	30	20	50	2	2
III	CHE DMI 302 & CHE IDMI 304	Basic Analytical Chemistry	30	20	50	2	2
IV	CHE DMI 402 & CHE IDMI 404	Chemical and Phase Equilibria, Solutions and Colligative Properties	30	20	50	2	2
V	CHE DMI 502 & CHE IDMI 504	Advanced Analytical Chemistry	30	20	50	2	2
VI	CHE DMI 602 & CHE IDMI 605	Organic Spectroscopy	30	20	50	2	2

The I-VI Minor disciplinary/multidisciplinary paper may be substituted by the following additional Minor papers subject to the availability of the Teacher and class load of the discipline/teacher in any semester.

Additional Course:

CHE DMI 102/ CHE IDMI 104: IT Skill for Chemist

CHE DMI 202/ CHE IDMI 204: Green Methods in Chemistry

CHE DMI 302/ CHE IDMI 304: Basic of Nanomaterials

CHE DMI 402/ CHE IDMI 404: Crystalline Materials and Properties

CHE DMI 502/ CHE IDMI 504: Inorganic Materials of Industrial Importance

CHE DMI 602/ CHE IDMI 605: Basic of Drug Design & Medicinal Chemistry

Disciplinary Minor /Inter-disciplinary Minor

SEMESTER – I

CHE DMI 102/ CHE IDMI 104: States of Matter and Colloidal State

SYLLABUS

Unit – I: Gaseous State

Postulates of Kinetic Theory of Gases and derivation of the kinetic gas equation.

Behavior of real gases: Deviations from ideal gas behavior, compressibility factor and its variation with pressure for different gases. Causes of deviation from ideal behavior; van der Waals equation of state, its derivation and application in explaining real gas behavior, mention of other equations of state (Berthelot, Dietrici); virial equation of state; van der Waals equation expressed in virial form and calculation of Boyle temperature. Isotherms of real gases and their comparison with van der Waals isotherms, continuity of states, critical state, relation between critical constants and van der Waals constants, law of corresponding states.

Maxwell Boltzmann distribution laws of molecular velocity and molecular energies (graphic representation – derivation not required) and its use in evaluating molecular velocities (average, root mean square, and most probable) and average kinetic energy, law of equipartition of energy, degrees of freedom and molecular basis of heat capacities.

Collision frequency, collision diameter, and mean free path including their temperature and pressure dependence; viscosity of gases, relation between mean free path and coefficient of viscosity; calculation of collision diameter from coefficient of viscosity; variation of viscosity of gases with temperature and pressure.

Unit – II: Solid State

Nature of the solid state, definition of space lattice, unit cell; laws of crystallography – (i) law of constancy of interfacial angles, (ii) law of rational indices (Miller indices) and, (iii) law of symmetry, elementary ideas of symmetry, symmetry elements and symmetry operations. qualitative idea of point and space groups, seven crystal systems and fourteen Bravais lattices; X-ray diffraction, Bragg's law, a simple account of rotating crystal method and powder pattern method. Analysis of powder diffraction patterns of NaCl, CsCl and KCl. Defects in crystals. Glasses and liquid crystals.

Unit – III: Liquid and Colloidal States

Qualitative treatment of the structure of the liquid state; Radial distribution function; physical properties of liquids; vapor pressure, surface tension and coefficient of viscosity, and their determination. Effect of addition of various solutes on surface tension and viscosity. Explanation of cleansing action of detergents. Temperature variation of viscosity of liquids and comparison with that of gases. Qualitative discussion of structure of water.

Definition of colloids, classification of colloids. Solids in liquids (sols); properties– kinetic, optical and electrical, stability of colloids, protective action; Hardy-Schulze law, gold number. Liquids in liquids (Emulsions): types of emulsions (micelles and reverse micelles), preparation, emulsifier. Liquid in solid (gels): classification, preparation, and properties, general application of colloids.

SEMESTER – II

PAPER CODE: CHE DMI 202/ CHE IDMI 204: Chemistry in Daily Life

SYLLABUS

Unit I: Chemicals in the Environment

Introduction, General mechanisms that occur after the discharge of a Chemical into the Environment, Sources: Point and Non-Point Sources of Pollutants, Atmospheric pollutants (benzene, acid deposits-NO_x and SO_x, Ozone, Radioactive pollutants and their effects, Photochemical Pollutants). Water Pollution and common disinfectants (KMnO4, Chlorination, Ozone, UV light), Industrials Chemicals and their Impacts on Environment.

Unit II Agrochemicals

Demand and supply gap of Food and improving the productivity, Introduction to agrochemicals (insecticides, fungicides, and herbicides), History of agrochemicals and Lead optimization, and Agrochemicals utilized in Modern days and recent markets.

Unit III Food Chemistry

Major Food Components (Major Food Components: Carbohydrates, Lipid, Proteins, and enzymes: Structures, and properties), Minor Food Components: Vitamins, Minerals, Colorants, Flavors, Food Additives etc.

Unit IV Household Chemistry

FUELS: Solid (coal, coke, and charcoal), liquid (kerosene oil, petrol and diesel oil) and gas (LPG and CNG). Non-conventional sources of energy. ACIDS, BASES AND SALTS: Properties and uses of sulphuric acid, hydrochloric acid and nitric acid. Properties and uses of sodium carbonate, sodium bicarbonate, baking powder, boric acid, borax and bleaching powder. Useful Organic Products: Vinegar, Ethyl alcohol, and DRUGS: Antiseptics and disinfectants.

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SEMESTER – III

PAPER CODE: CHE DMI 302/ CHE IDMI 304: Basic Analytical Chemistry

SYLLABUS

Unit – I: Qualitative and quantitative aspects of analysis

Sampling, evaluation of analytical data, errors, accuracy and precision, methods of their expression, normal law of distribution if indeterminate errors, statistical test of data; F, Q and t test, rejection of data, and confidence intervals.

Qualitative Analysis of Inorganic Radicals

Introduction to salt analysis, dry and wet test for acid and basic radicals, Principle and chemistry of qualitative analysis of inorganic salt; chemistry involved in qualitative analysis of mixture containing interfering radicals and insolubles.

Unit - II: Volumetric Titration

Standard solution, primary standard and secondary standard, titration, end point, indicator, concentration of standard solution- moles, Normality, molarity, Molality, parts per million(PPM), volumetric calculation, acid base titration and use of indicators, titration curves for strong acid vs strong base, weak acid with strong base, weak base with strong acid, theory of acid base indicator, Redox titration- titration of Mohr salt against $KMnO_4$, Titration of Oxalic acid against $KMnO_4$, Titration of $FeSO_4$ against $K_2Cr_2O_7$, Iodometric and iodimetric titration, Internal and external indicator, complexometric titration- EDTA titration, Eriochrome black T indicator, complexometric titration curve, direct and back titration, masking and demasking of cations, precaution in volumetric titration.

Unit – III: Basic techniques of Spectroscopy

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law in UV-Visible Spectrometry, Infrared Spectrometry.

Flame Atomic Absorption and Emission Spectrometry: Basic principles of instrumentation (choice of source, monochromator, detector, choice of flame and Burner designs. Techniques of atomization and sample introduction; Method of background correction, sources of chemical interferences and their method of removal. Techniques for the quantitative estimation of trace level of metal ions from water samples.

SEMESTER – IV

PAPER CODE: CHE DMI 402/CHE IDMI 404: Chemical and Phase Equilibria, Solutions and Colligative Properties

SYLLABUS

Unit – I: Chemical Equilibrium

Criteria of thermodynamic equilibrium, degree of advancement of reaction, chemical equilibria in ideal gases. Thermodynamic derivation of relation between Gibbs free energy of reaction and reaction quotient. Coupling of exoergic and endoergic reactions. Equilibrium constants and their quantitative dependence on temperature, pressure and concentration; thermodynamic derivation of relations between the various equilibrium constants *Kp*, *Kc* and *Kx*. Le Chatelier principle (quantitative treatment); equilibrium between ideal gases and a pure condensed phase.

Unit – I: Phase Equilibrium and Phase Transformation

Concept of phases, components and degrees of freedom, derivation of Gibbs Phase Rule for nonreactive and reactive systems; Phase diagrams with applications for one-component systems (water and sulfur) and two component systems involving eutectics, congruent, incongruent melting points and solid solution (lead-silver, FeCl3-H2O and Na-K *etc*.).

Three Component System: Graphical representation of three component system; system of three liquids: having partial miscibility.

Type-I Formation of one pair of partially miscible liquids, **Type-II** Formation of two pairs of partially miscible liquids, **Type-III** Formation of three pairs of partially miscible liquids

Stability of phases; Clapeyron equation; Clasius-Clapeyron equation and its applications to solid-liquid, liquid-vapor and solid-vapor equilibria. Thermodynamics of phase transition; classification of phases - bubbles, cavities and droplets-Kelvin equation.

Unit – III: Solutions and Colligative Properties

The chemical potential of liquids; ideal solutions; lowering of vapor pressure, Raoult's and Henry's Laws and their applications. Excess thermodynamic functions.

Thermodynamic derivation using chemical potential to derive relations between the four colligative properties [(i) relative lowering of vapor pressure, (ii) elevation of boiling point, (iii) Depression of freezing point, (iv) osmotic pressure] and amount of solute. Applications in calculating molar masses of normal, dissociated, and associated solutes in solution.

Binary solutions: Gibbs-Duhem-Margules equation, its derivation and applications to fractional distillation of binary miscible liquids (ideal and non-ideal), vapor pressure-composition and temperature-composition curves of ideal and non-ideal solution; distillation of solution, Lever rule, azeotropes. Partial miscibility of liquids, CST, miscible pairs, Immiscibility of liquids – Principle of steam distillation.

Nernst distribution law: its derivation and applications.

SEMESTER – V

PAPER CODE: CHE DMI 502/ CHE IDMI 504: Advanced Analytical Chemistry

SYLLABUS

Unit – I: Separation techniques:

Solvent extraction: Classification, principle and efficiency of the technique. Distribution Coefficient, distribution ratio, percent extracted.
Mechanism of extraction: extraction by solvation and chelation.
Technique of extraction: batch, continuous and counter current extractions.
Qualitative and quantitative aspects of solvent extraction: extraction of metal ions from aqueous solution, extraction of organic species from the aqueous and nonaqueous media.

***Ion-exchange*:** Column, ion-exchange chromatography etc. Determination of ion exchange capacity of anion / cation exchange resin (using batch procedure if use of column is not feasible).

Chromatography: Classification, principle and efficiency of the technique.
Mechanism of separation: adsorption, partition & ion exchange.
Development of chromatograms: frontal, elution and displacement methods.
Qualitative and quantitative aspects of chromatographic methods of analysis: IC, GLC, GPC, TLC and HPLC.

Gas Chromatography: retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Unit – II: Gravimetric analysis:

Basic principle of gravimetry, preparation of solution, precipitation, condition for analytical precipitation, saturation, supersaturation, nucleation, von weimarn ratio, digestion of the precipitate, Ostwald ripening, colloidal, peptization, impurities in precipitates, occlusion, inclusion, surface adsorption, postprecipitation, washing and filtering the precipitates, drying the precipitate, gravimetric calculation

Unit – III: Thermal and Electroanalytical analysis:

Theory of thermogravimetry (TG), basic principle of instrumentation. Techniques for quantitative estimation of Ca and Mg from their mixture. 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.

Classification of electroanalytical methods, basic principle of pH metric, potentiometric and conductometric titrations. Techniques used for the determination of equivalence points. Techniques used for the determination of pK_a values.

SEMESTER – VI

PAPER CODE: CHE DMI 602/ CH IDMI 605: Organic Spectroscopy

SYLLABUS

Unit I: Basics of Organic Spectroscopy and Ultraviolet Spectroscopy

Electromagnetic radiations: Types of molecular energy and molecular 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.

Unit II: Infrared Spectroscopy

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

Unit III: 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). 13C NMR, Heteronuclear coupling, Chemical shifts, coupling constant,

Unit IV: Mass Spectrometry

Molecular ion peak, base peak, isotopic abundance, 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

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CHE DMI 102/ CH IDMI 103: IT Skill for Chemists

Unit – I: Mathematics

Fundamentals, mathematical functions, polynomial expressions, logarithms, the exponential function, units of a measurement, interconversion of units, constants and variables, equation of a straight line, plotting graphs.

Uncertainty in experimental techniques: Displaying uncertainties, measurements in chemistry, decimal places, significant figures, combining quantities.

Uncertainty in measurement: types of uncertainties, combining uncertainties. Statistical treatment. Mean, standard deviation, relative error. Data reduction and the propagation of errors. Graphical and numerical data reduction. Numerical curve fitting: the method of least squares (regression).

Algebraic operations on real scalar variables (e.g. manipulation of van der Waals equation in different forms).Roots of quadratic equations analytically and iteratively (e.g. pH of a weak acid). Numerical methods of finding roots (Newton-Raphson, binary –bisection, e.g. pH of a weak acid not ignoring the ionization of water, volume of a van der Waals gas, equilibrium constant expressions).

Differential calculus: The tangent line and the derivative of a function, numerical differentiation (e.g., change in pressure for small change in volume of a van der Waals gas, potentiometric titrations).

Numerical integration (Trapezoidal and Simpson's rule, e.g. entropy/enthalpy change from heat capacity data).

Unit – II: Introductory writing activities & Handling numeric data

Introduction to word processor and structure drawing (ChemSketch) software. Incorporating chemical structures, chemical equations, expressions from chemistry (e.g. Maxwell-Boltzmann distribution law, Bragg's law, van der Waals equation, etc.) into word processing documents.

Spreadsheet software (Excel), creating a spreadsheet, entering and formatting information, basic functions and formulae, creating charts, tables and graphs. Incorporating tables and graphs into word processing documents. Simple calculations, plotting graphs using a spreadsheet (Planck's distribution law, radial distribution curves for hydrogenic orbitals, gas kinetic theory- Maxwell-Boltzmann distribution curves as function of temperature and molecular weight), spectral data, pressure-volume curves of van der Waals gas (van der Waals isotherms), data from phase equilibria studies. Graphical solution of equations.

Unit – III: Numeric modeling & Statistical Analysis

Simulation of pH metric titration curves. Excel functions LINEST and Least Squares. Numerical curve fitting, linear regression (rate constants from concentration-time data, molar extinction coefficients from absorbance data), numerical differentiation (e.g. handling data from potentiometric and pH metric titrations, pK_a of weak acid), integration (e.g. entropy/enthalpy change from heat capacity data).

Statistical Analysis: Gaussian distribution and Errors in measurements and their effect on data sets. Descriptive statistics using Excel. Statistical significance testing: The *t* test. The *F* test.

Presentation: Presentation graphics

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CHE DMI 202/ CHE IDMI 204: Green Methods in Chemistry

Unit – I: Short Introduction to Green Chemistry

What is Green Chemistry? Need for Green Chemistry. Goals of Green Chemistry. Limitations/ Obstacles in the pursuit of the goals of Green Chemistry.

Unit – II: Principles

Tools of Green chemistry, Twelve principles of Green Chemistry, with examples. Designing a Green Synthesis using these principles; Prevention of Waste/ byproducts; maximum incorporation of the materials used in the process into the final products (Atom Economy); prevention/ minimization of hazardous/ toxic products; designing safer chemicals: green solvents, solventless processes, immobilized solvents and ionic liquids; energy requirements for reactions - use of microwaves, ultrasonic energy; selection of starting materials; avoidance of unnecessary derivatization – careful use of blocking/protecting groups; use of catalytic reagents (wherever possible) in preference to stoichiometric reagents; designing of biodegradable products; prevention of chemical accidents; strengthening/ development of analytical techniques to prevent and minimize the generation of hazardous substances in chemical processes.

Unit – III: Examples of Green Synthesis/ Reactions

1. Green Synthesis of the following compounds: adipic acid, catechol, BHT, methyl methacrylate, urethane, aromatic amines (4-aminodiphenylamine), benzyl bromide, acetaldehyde, citral, ibuprofen, paracetamol, furfural.
2. Microwave assisted reactions in water: Hofmann Elimination, Hydrolysis (of benzyl chloride, benzamide, n-phenyl benzamide, methylbenzoate to benzole acid), Oxidation (of toluene, alcohols).
3. Microwave assisted reactions in organic solvents: Esterification, Fries rearrangement, Orthoester Claisen Rearrangement, Diels-Alder Reaction, Decarboxylation.
4. Microwave assisted solid state reactions: Deacetylation, Deprotection. Saponification of esters, Alkylation of reactive methylene compounds, reductions, synthesis of nitriles from aldehydes; anhydrides from dicarboxylic acid; pyrimidine and pyridine derivatives; 1,2-dihydrotriazine derivatives; benzimidazoles.
5. Ultrasound assisted reactions: Esterification, saponification, substitution reactions, Alkylations, oxidation, reduction, coupling reaction, Cannizaro reaction, Strecker synthesis, Reformatsky reaction.

Unit – IV: Future Trends in Green Chemistry

Oxidation reagents and catalysts; Biomimetic, multifunctional reagents; Combinatorial green chemistry; Proliferation of solventless reactions; oncovalent derivatization; Green chemistry in sustainable development

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CHE DMI T 302/ CH IDMI 304: Basic of Nanomaterials

Unit – I: Introduction and Classification

What is nanotechnology?; Why nano? Classification of nanostructures, nanoscale architecture; summary of the electronic properties of atoms and solids; the isolated atom, bonding between atoms, giant molecular solids, the free electron model and energy bands of crystalline solids, periodicity of crystal lattices; electronic conduction; effects of the nanometre length scale, changes to the system total energy, changes to the system structure; how nanoscale dimensions affect properties. (electronic conduction, system classification confined to one, two or three dimension and their effect on properties).

Unit – II: Properties & Synthesis of Nanomaterials

Properties: Introductory discussion of size and shape dependable properties of nanomaterials like melting point, magnetism, optical, conductivity (conductor and semi-conductivity), catalytic and electrochemical aspect.

Synthesis: Common methods of top down and bottom approaches of the preparation of nanomaterials. Special interest on the synthesis of metal nanoparticles, metal oxides, and carbon nanotube (CNT) *etc*. A brief discussion of biological synthesis of nanomaterials.

Unit – IV: Characterization & Applications of Nanomaterials

Characterization: A brief historical overview of common instrumental techniques used for characterization of nanomaterials such as, X-ray diffraction, electron microscopy (SEM, TEM, including EDX technique), XPS with respect to working principle, instrumentation and applications. Differential scanning calorimeter (DSC), Thermogravimetric / Diffferential (TG/DTA), UV-Visible Spectrophotometer, and FTIR –Principle and Applications.

Applications: Use of nanomaterials in daily life with examples (solar cell, GMR read heads, NEMS goniometers, health care, energy materials, *etc*). Societal aspects of nanotechnology: health, environment, hype and reality.

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CHE DMI 402/ CHE IDMI 404: Crystalline Materials and Properties

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Unit – I: Introduction, Bonding & Crystal structure of the Materials

Introduction: Crystalline and non-crystalline solids; space lattice and primitive and non-primitive lattice, crystal structure, unit cell, symmetry in crystal, seven crystal system, Bravais lattice, a qualitative ideas of point and space group; crystal planes and Miller indices, reciprocal lattice.
Cubic lattice: lattice point in cubic crystals, coordination number, Packing density, separation between crystal planes

Bonding and Crystal Structure of Crystalline Materials

Closed packed structure- hcp and ccp, packing efficiency, voids, limiting radius ratio; description of solid structure of rack salt (NaCl), Wurzite and zinc blend of ZnS, Fluoride (CaF_2) and antifluoride (Na_2O), Rutile (TiO_2).
Bonding between atoms in solid: ionic bonds, covalent bonds, metallic bonds, van der Waals bonds; cohesive energy of an ionic crystal, Madelung constant and lattice energy.

Unit – II: Determination of Crystal Structure

X-ray diffraction by crystal, Bragg's law, a simple description of rotating crystal method and powder pattern methods. Analysis of powder pattern of simple cubic systems.
A brief overview of determination of crystal structure by electron microscope (TEM, SAED, and HRTEM)

Unit – III: Thermal, Electrical and Magnetic Properties of Solids

Thermal Properties: Specific heat of solids, classical theory – Dulong-Petit's law, Einstein-Debye theory, vibrational modes of one dimensional lattice – dispersion relation and Brillouin zones.
Electronic Properties: Free electron theory of metals; solution of one dimensional Schrödinger equation in constant potential; density of state; Fermi energy; Energy band in a solid, explanations of Kronig-Penney model (without derivation), refinement of simple band formation in solid, *k*-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, *p*-*n* junctions. Hall effect- definition, Hall potential Hall coefficient. Superconductivity- qualitative discussion, critical temperature, Meissner effect, and Josephson Tunnelling.

Magnetic Properties of Solids: Concept of dia- para- and ferro- magnetism; magnetic moment due to orbital and spin motion of electron, effect of temperature, Langevin's theory of dia- and para- magnetism; Curie-Weiss law, qualitative description of ferro-magnetism (magnetic domains), B-H curve, hysteresis loop, retentivity, coercivity, hysteresis loss, soft and hard magnets.

CHE DMI 502/ CHE IDMI 504: Inorganic Materials of Industrial Importance

Unit – I: Silicate Industries

Glass: Glassy state and its properties, classification (silicate and non-silicate glasses). Manufacture and processing of glass. Composition and properties of the following types of glasses: Soda lime glass, lead glass, armoured glass, safety glass, borosilicate glass, fluorosilicate, coloured glass, photosensitive glass.
Ceramics: Important clays and feldspar, ceramic, their types and manufacture. High technology ceramics and their applications, superconducting and semiconducting oxides, fullerenes carbon nanotubes and carbon fibre.
Cements: Classification of cement, ingredients and their role, Manufacture of cement and the setting process, quick setting cements.

Unit – II: Fertilizer & Surface Coatings

Different types of fertilizers. Manufacture of the following fertilizers: Urea, ammonium nitrate, calcium ammonium nitrate, ammonium phosphates; polyphosphate, superphosphate, compound and mixed fertilizers, potassium chloride, potassium sulphate.

Objectives of coatings surfaces, preliminary treatment of surface, classification of surface coatings. Paints and pigments-formulation, composition and related properties. Oil paint, Vehicle, modified oils, Pigments, toners and lakes pigments, Fillers, Thinners, Enamels, emulsifying agents. Special paints (Heat retardant, Fire retardant, Eco-friendly paint, Plastic paint), Dyes, Wax polishing, Water and Oil paints, additives, Metallic coatings (electrolytic and electroless), metal spraying and anodizing.

Unit – III: Batteries & Alloys

Primary and secondary batteries, battery components and their role, Characteristics of Battery. Working of following batteries: Pb acid, Li-Battery, Solid state electrolyte battery. Fuel cells, Solar cell and polymer cell.
Classification of alloys, ferrous and non-ferrous alloys, Specific properties of elements in alloys. Manufacture of Steel (removal of silicon decarbonization, demanganization, desulphurization dephosphorisation) and surface treatment (argon treatment, heat treatment, nitriding, carburizing). Composition and properties of different types of steels.

Unit – IV: Catalysis & Chemical explosives

General principles and properties of catalysts, homogenous catalysis (catalytic steps and examples) and heterogenous catalysis (catalytic steps and examples) and their industrial applications, Deactivation or regeneration of catalysts.
Phase transfer catalysts, application of zeolites as catalysts.
Origin of explosive properties in organic compounds, preparation and explosive properties of lead azide, PETN, cyclonite (RDX). Introduction to rocket propellants.

CHE DMI 602/ CHE IDMI 605: Basics of Drug Design & Medicinal Chemistry

Unit – I: Basic Concept of Drug Design & Physiochemical Factors

Introduction; Basics of drug design; analog and Prodrug; Cocept of lead; Factors governing drug design; Rational approach to drug design.

Physical-Chemical factors and biological activities; Factors governing ability of drug to reach active site.

Unit – II: Molecular Modeling & Ligand Design Concept

Concept of structure of drug molecules and its optimization; Molecular modeling and drug design; Basic concept of Protein and its structure; Structure based drug design; Ligand receptor recognition; Active site of a target molecules; Characterization of site and design of ligands.

Unit – III: Types of Drugs

Concept of Analgesics drug; Synthesis and use of analgesics drugs: Paracetamol, Phenacetine, Acetanilide, Aspirin, Salol, Cinchophene, and Phenazone.

Antimalerial Drugs: Synthesis and use of Chloroquine phosphate.

Antibacterial Drugs & Properties:

Sulphonamide drugs: Synthesis and use of Sulphonamide drugs: Sulphanilide, Sulphapyridine, Sulphathiazole, Sulphadiazine, Antibacterial properties.

Concept of Antibiotics with its application.

Unit – IV: Herbal medicine

Herbal Drug: Its importance

Ethanobotanical survey methods; introduction to ayurveda, pharmacopia; plants as source of drugs; Indian medicinal plants and uses - Tulasi, Neem, Pili, Mango, Sarpagandhi, Gulbakavali, Shyma Haldi, Vanchana, Safed Musli, Aswagandha, Satavar, Pipalendi, Digitalis, Senna, Clove, Cardamom, Plantago, *Artemisia annua*, *Coleus forskoli*, Aloe

Patal Kumhda, Banpyaz.

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Paper in Chemistry:

Semester	Paper Code	Course Title	Credit
I	CHE VOT 105	Basic Concepts of Physical Chemistry Experiments, Energy, and Environment	02
	CHE VOP 106	Vocational Chemistry Practical – I	02
II	CHE VOT 205	Cosmetics, Perfumes, & Pharmaceutical Chemistry	02
	CHE VOP/I 206	Vocational Chemistry Practical – II /Internship (Industrial visit)	02
III	CHE VOT 305	Cement, Extraction of Ores, Pesticides & Fuel Chemistry	02
	CHE VOP 306	Vocational Chemistry Practical – III	02
IV	CHE VOT 405	Techniques of Instrumental Analysis (Principles and Applications of X-ray diffraction, FT-IR, UV, GCMS, LCMS etc.)	02
	CHE VOP/I 406	Hands Training on Instrument	02

CHE VOT 105: Basic Concepts of Physical Chemistry Experiments, Energy, and Environment

Unit I- Safety Measures in Chemical Laboratory and Experiment Execution

Introduction to chemical laboratory: general guidelines, cleanness, reagents, glasswares, and equipments; safety symbols and regulations in chemical laboratory. Materials Safety Data Sheet (MSDS). Globally CAS registry number. Global overview of chemical regulations in India. Fundamentals units of measure.

Analytical balance and weights: general purpose chemical balance, electronic balance, analytical weight box and classification, calibration of weights and handling of electronic balance. Handling of laboratory apparatus and hazardous chemicals. Calibration of glassware (pipette, burette, etc.).

Types of solutions: mole and mole concept, equivalent weight, formula weight. Expression of concentration, molarity (M), molality (m), mole fraction, normality (N); weight, volume, and weight-to-volume ratios; parts per million (ppm), parts per billion (ppb).

Preparation of an experiment: Literature Work; Execution of an Experiment (general advice, data collection, bias, safety); Recording of Experimental Data (what to record, computer files and disks); Reporting of works (Style, format, tables, figures,) in term of Introduction, Experimental Methods, Result and Discussion. Ethics, References.

Unit –II: Treatment of Experimental Data

Significant figures, accuracy and precision in calculations. Uncertainties (error) in Data and Results, classification of errors, minimizations of errors, distribution of random errors, propagation of error. Reliability of Results, Confidence Interval, Rejection of data (t-test, F-test, and Q-test), Mean and Standard Deviations, Correlation and Regression,

Use of Computer: Excel spread sheet, data entry and manipulation, formula entry and addressing, significance test, Graph plotting, curve fitting (linear and non-linear), and its analysis (including origin software), and advanced spreadsheet tools.

Microsoft power point presentation, Molecule design and its properties determination using computational softwares, Introduction of various computational softwares for chemical sciences.

Unit III- Energy and Environment

Energy, Solar energy, Coal, petroleum and natural gas, Hydro-power, wind power, ocean energy, geothermal energy, Nuclear energy: Fission & Fusion, Fuel cells, & Battery.

Ecosystem, Environmental and its segments, Green house effect, Global warming, Air pollution, Water pollution, Soil pollution, Industrial waste, Control measures of environmental pollution. Plastic pollutants and remedies.

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CHE VOP 106: Vocational Chemistry Practical – 1

1. Calibration of weights and glasswares.
2. Preparation of solutions for given concentrations.
3. Measurement of pH of tape water.
4. Measurement of conductivity of given unknown solution.
5. Determination of Biological Oxygen Demand (BOD)
6. Determination of Chemical Oxygen Demand (COD)
7. Measurement of chloride, sulfate and salinity of water samples by simple titration methods ($AgNO_3$ and potassium chromate)
8. Programming of computer applications.
9. Graph plotting with data provided.
10. ***Some others experiments in the class if permit.***

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CHE VOT 205: Cosmetics, Perfumes & Pharmaceutical Chemistry

Unit – I: Introduction of Cosmetics & perfumes chemistry

History of Cosmetics & perfumes chemistry, a general study including preparation and uses of the following: Hair dye, hair spray, shampoo, suntan lotions, face powder, lipsticks, talcum powder, nail enamel, creams (cold, vanishing and shaving creams), antiperspirants and artificial flavours. Essential oils and their importance in cosmetic industries with reference to Eugenol, Geraniol, sandalwood oil, eucalyptus, rose oil, 2-phenyl ethyl alcohol, Jasmone, Civetone, Muscone.

Unit – II: Synthesis procedure

1. Preparation of talcum powder.
2. Preparation of shampoo.
3. Preparation of enamels.
4. Preparation of hair remover.
5. Preparation of face cream.
6. Preparation of nail polish and nail polish remover.

Unit – III: Drugs & Pharmaceuticals

Drug discovery, design and development; Basic Retrosynthetic approach. Synthesis of the representative drugs of the following classes: analgesics agents, antipyretic agents, anti-inflammatory agents (Aspirin, paracetamol, lbuprofen); antibiotics (Chloramphenicol); antibacterial and antifungal agents (Sulphonamides; Sulphanethoxazol, Sulphacetamide, Trimethoprim); antiviral agents (Acyclovir), Central Nervous System agents (Phenobarbital, Diazepam), Cardiovascular (Glyceryl trinitrate), antilaprosy (Dapsone), HIV-AIDS related drugs (AZT- Zidovudine).

Fermentation: Aerobic and anaerobic fermentation. Production of (i) Ethyl alcohol and citric acid, (ii) Antibiotics; Penicillin, Cephalosporin, Chloromycetin and Streptomycin, (iii) Lysine, Glutamic acid, Vitamin B2, Vitamin B12 and Vitamin C.

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CHE VOP/I 206: Vocational Chemistry Practical – II

(a) Drawing of different organic molecules using ChemDraw and ChemSketech software.
(b) Synthesis and characterization of following drugs:

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

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CHE VOT 305: Cement & Ores, Pesticide & Fuel Chemistry

Unit – I: Cement & Extraction of Ores

History of binding materials and Cement, Classification of Cement Binders, Lime as Binder, cement and its importance in construction, History of Cement manufacturing process, material composition of cement, various unit operation of cement manufacture in India, Sources of cement raw materials, Calcareous Materials: Source of Lime, Limestone, Chalk, Marl.

Argillaceous raw materials: Source of Silica, Alumina, Iron Oxide, Shale and effect of coalash.

Alternate Raw Materials: Industrial waste, types of industrial waste use as alternative raw materials for cement manufacture: fly ash, blast furnace slag, LD slag, red mud, lime sludge, phosphogypsum, jerosite, lead and zinc slag, kimberlight rejects, marble slurry, mines rejects, cement kiln dust

Type of Cements: Ordinary Port Land Cement with different grade, Portland Pozzolana Cement, Portland Slag Cement, Ordinary & Rapid Hardening Portland cement, Sulphate Resisting Portland cement, White Portland cement, Coloured Portland cement, Water Repellent and Hydrophobic Portland cement , Masonry cement, Super Sulphate cements, High Early Strength cement.

Additives and Gypsum: Origin and occurrences, distribution/ availability in India, Physical and Chemical Characteristics of various additives such as Bauxite, Iron Ore, Laterite, and gypsum.

Extraction of Ores: Bauxite, Iron, etc.

Unit – II: Pesticide Chemistry & Preparation Procedure

General introduction of Chemical toxicology and pesticides (natural and synthetic), benefits and adverse effects, changing concepts of pesticides, structure activity relationship, synthesis and technical manufacture and uses of representative pesticides in the following classes: Organochlorines (DDT, Gammexene,); Organophosphates (Malathion, Parathion); Carbamates (Carbofuran and carbaryl); Quinones (Chloranil), Anilides (Alachlor and Butachlor).

Unit –III: Fuel Chemistry

Review of energy sources (renewable and non-renewable). Classification of fuels and their calorific value. ***Coal:*** Uses of coal (fuel and nonfuel) in various industries, its composition, carbonization of coal. Coal gas, producer gas and water gas—composition and uses. Fractionation of coal tar, uses of coal tar bases chemicals, requisites of a good metallurgical coke, Coal gasification (Hydro gasification and Catalytic gasification), Coal liquefaction and Solvent Refining.

Petroleum and Petrochemical Industry: Composition of crude petroleum, Refining and different types of petroleum products and their applications.

Fractional Distillation (Principle and process), Cracking (Thermal and catalytic cracking), Reforming Petroleum and non-petroleum fuels (LPG, CNG, LNG, bio-gas, fuels derived from biomass), fuel from waste, synthetic fuels (gaseous and liquids), clean fuels. Petrochemicals: Vinyl acetate, Propylene oxide, Isoprene, Butadiene, Toluene and its derivatives Xylene.

Lubricants: Classification of lubricants, lubricating oils (conducting and non-conducting) Solid and semisolid lubricants, synthetic lubricants.

Properties of lubricants (viscosity index, cloud point, pore point) and their determination.

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CHE VOP 306: Vocational Chemistry Practical – III

I. (i) Analysis of Ores: Felspar, bauxite, Rocks available in that region (At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session)

(ii) Determination of composition of dolomite (by complexometric titration).
(iii) Analysis of (Cu, Ni); (Cu, Zn) in alloy or synthetic samples.
(iv) Analysis of Cement: Determination of density, Determination of specific surface, Determination of setting time, Determination of soundness test by Le Chatelier Autoclave, Determination of compressive strength, Determination of drying shrinkage
(v) Preparation of pigment (zinc oxide).
(vi) Analysis of Soil sample, animal feeds, soil micronutrients, milk powder for Ca, Fe and P content.
(vii) Estimation of calcium, magnesium, phosphate, nitrate in fertilizer
(viii) Determination of pH of soil.

II. Separation Techniques

1. Chromatography:

(a) Separation of mixtures

i. Paper chromatographic separation of Fe^{3+}, Al^{3+}, and Cr^{3+}.
ii. Separation and identification of the monosaccharides present in the given mixture (glucose & fructose) by paper chromatography. Reporting the R_f values.

(b) Separate a mixture of Sudan yellow and Sudan Red by TLC technique and identify them on the basis of their R_f values.

(c) Chromatographic separation of the active ingredients of plants, flowers and juices by TLC

CHE VOT 405: Techniques of Instrumental Analysis

Unit – I: Basic Spectroscopy

Origin of spectra, interaction of radiation with matter, fundamental laws of spectroscopy and selection rules, validity of Beer-Lambert's law.

UV-Visible Spectrometry: Basic principles of instrumentation (choice of source, monochromator and detector) for single and double beam instrument;

Infrared Spectrometry: Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

Fluorescence Spectroscopy: Basic principles of fluorescence spectrophotometer, Basic principles of instrumentation (choice of source, monochromator & detector) for single and double beam instrument; sampling techniques.

NMR spectroscopy: Principle, Instrumentation, Chemical shift, Factors affecting chemical shift, Spin-coupling, Applications: ^{1}H-NMR spectroscopy and 13C-NMR

Unit – II: X-Ray Diffraction

Crystalline and non-crystalline solids; space lattice and primitive and non-primitive lattice, crystal structure, unit cell, symmetry in crystal, seven crystal system, Bravais lattice, a qualitative ideas of point and space group; crystal planes and Miller indices, reciprocal lattice.

X-ray diffraction by crystal, Bragg's law, a simple description of rotating crystal method and powder pattern methods. Analysis of powder pattern of simple cubic systems.

Unit – III: Mass spectroscopy & Chromatography

Mass spectroscopy: Making the gaseous molecule into an ion (electron impact, chemical ionization), Making liquids and solids into ions (electrospray, electrical discharge, laser desorption, fast atom bombardment), Separation of ions on basis of mass to charge ratio, Magnetic, Time of flight, Electric quadrupole. Resolution, time and multiple separations, Detection and interpretation (how this is linked to excitation).

Chromatography: Gas chromatography, liquid chromatography, supercritical fluids, Importance of column technology (packing, capillaries), Separation based on increasing number of factors (volatility, solubility, interactions with stationary phase, size, electrical field), Basic Instrumentation Principles of Gas Chromatography Mass Spectroscopy (GCMS) and Liquid Chromatography Mass Spectroscopy (LCMS) and Applications.

CHE VOT/I 406: Hands Training of Instruments

1. Determination of λ_{max} of different standard solutions by UV-vis spectroscopy measurement.
2. Determination of λ_{max} by excitation of a particular wavelength of different standard solutions by fluorescence spectroscopy measurement.
3. Data collection, graph plot and analysis of known/unknown samples by powder X-ray diffraction.
4. Sample analysis of different organic compounds by GCMS and LCMS.

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