

BANASTHALI VIDYAPITH

Master of Science (Chemistry)



Curriculum Structure

First Semester Examination, December 2020
Second Semester Examination, April/May 2021
Third Semester Examination, December 2021
Fourth Semester Examination, April/May 2022

BANASTHALI VIDYAPITH
P.O. BANASTHALI VIDYAPITH
(Rajasthan)-304022

July, 2020

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No. F. 9-6/81-U.3

**Government of India
Ministry of Education and Culture
(Department of Education)**

New Delhi, the 25th October, 1983

NOTIFICATION

In exercise of the powers conferred by Section 3 of the University Grants Commission Act, 1956 (3 of 1956) the Central Government, on the advice of the Commission, hereby declare that Banasthali Vidyapith, P. O. Banasthali Vidyapith, (Rajasthan) shall be deemed to be a University for the purpose of the aforesaid Act.

Sd/-

(M. R. Kolhatkar)

Joint Secretary of the Government of India

NOTICE

Changes in Bye-laws/Syllabi and Books may from time to time be made by amendment or remaking, and a Candidate shall, except in so far as the Vidyapith determines otherwise, comply with any change that applies to years she has not completed at the time of change.

MASTER OF SCIENCE

14 (HE) B2:

- I. The courses of study for M. Sc. Examination shall extend over a period of two years divided into four semesters with an examination at the end of each semester. First and Second semester examinations in the First Year and the Third and Fourth semester examinations in the Second year.
- II. First and Third Semester examinations will normally be held in the month of December and Second and Fourth Semester examinations will normally be held in April/May every year.
- III. The candidate can offer M. Sc. Examination in one of the following subjects –
 - (i) Physics
 - (ii) Chemistry
 - (iii) Pharmaceutical Chemistry
 - (iv) Bio-science
 - (v) Bio-technology
 - (vi) Applied Microbiology & Biotechnology
 - (vii) Bio-informatics
 - (viii) Computer Science
 - (ix) Electronics
 - (x) Mathematical Science
- IV. The Examination shall be conducted by means of continuous assessment / written papers / Practicals / Dissertations / Project Report/ Seminar wherever prescribed.
- V. The following shall be the Scheme of Examination:

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Programme Objectives

Banasthali Vidyapith's educational ideology, aims to nurture future scientist through all round development of the student personality by inculcating proper sense of values and knowledge besides maintaining a harmonious balance of spiritual and scientific values. In view of this, the program objective of department of chemistry aims:

- To impart critical thinking by providing them with a foundation in chemistry that stresses scientific reasoning.
- To provide a real sense of education by inculcating in them ethics and values.
- To demonstrate information literacy skill for acquiring the ability to synthesize, separate and characterize compounds using published reactions, standard laboratory equipment, and modern instrumentation as a student and as a lifelong learner.
- To provide a foundation to carry accurate quantitative and qualitative measurements with an understanding of the theory and draw useful conclusion.
- To impart basic technical skills to solve pertaining problems independently, in concerned or interdisciplinary subjects.
- To create an awareness regarding effective and safe use of chemicals.

Programme Outcomes

- PO1:** Chemistry knowledge: Develop an insight of the core and importance of chemistry for society and individual well being
- PO2:** Planning ability: Acquire the skills of planning and conducting advanced chemical experiments and applying structural-chemical characterization techniques
- PO3:** Problem analysis: Identify, formulate, research literature, and analyze various analytical and experimental techniques taught during the course, for solving problems and make reasonable conclusions. The graduates should be able to systematically break up complex problems in realizable steps and solve them problems reaching substantiated conclusions
- PO4:** Communication: Communicate both written and oral, for specialized and non-specialized audiences
- PO5:** Modern tool usage: Use modern instrument and methods for dealing with structural problem taught during the course besides understanding its limitations. The graduate will be able to use modern tools, software, equipment etc. to analyze and obtain solution to the problems
- PO6:** Professional identity: Work as a Chemistry professional, and qualify for training as scientific researcher. Altitude of Professionalism to function effectively in the complex modern work environment /society with the ability to assume professional leadership roles and achieve professional understanding and appreciation of ethical behavior, social responsibility and diversity, both as individuals and in team environments. Explore new areas of research in both chemistry and allied fields of science and technology
- PO7:** Environment and sustainability: The graduates should practice their profession considering environmental protection and sustainability

- PO8:** Ethics: Honor the hard work of chemists, problem faced and how they surpassed the problem while performing novel experimental techniques and also get an understanding of harmful effects of chemicals and their necessity to dump them safely for individual and social well being
- PO9:** Chemist and society: The students will be able to study the impact of process industry on the global, economic, and societal context
- PO10:** Life-long learning: Longitude of not only opening careers in the branch in the concerned subject but also recognize the application of chemistry in context of problem in environmental, food processing, pharmaceutical, biochemical, agriculture, fuels and chemicals, textile processing, mining and many other industries and will be able to apply new innovative and novel approach to solve them.

Curriculum Structure

Master of Science (Chemistry)

First Year

Semester - I

Course Code	Course Name	L	T	P	C*
CHEM 401	Analytical Chemistry	4	0	0	4
CHEM 405	Inorganic Chemistry	4	0	0	4
CHEM 406	Organic Chemistry	4	0	0	4
CHEM 408	Physical Chemistry	4	0	0	4
MATH 407	Mathematics for Chemists	4	0	0	4
CHEM 402L	Chemistry Lab - I	0	0	12	6
Semester Total:		20	0	12	26

Semester - II

Course Code	Course Name	L	T	P	C*
CHEM 412	Special Topics in Physical Chemistry	4	0	0	4
CHEM 407	Organic Reaction Mechanism	4	0	0	4
CHEM 411	Photo Inorganic Chemistry	4	0	0	4
CHEM 409	Spectral Techniques in Inorganic Chemistry	4	0	0	4
CHEM 410	Spectroscopy	4	0	0	4
CHEM 403L	Chemistry Lab - II	0	0	12	6
Semester Total:		20	0	12	26

Second Year**Semester - III**

Course Code	Course Name	L	T	P	C*
CHEM 514	Bioinorganic and Bioorganic Chemistry	4	0	0	4
CHEM 516D	Literature Dissertation	0	0	8	4
CHEM 509	Organic Chemistry (Chemistry of Natural Products)	4	0	0	4
CHEM 521	Physical Spectroscopy	4	0	0	4
CHEM 505L	Chemistry Lab - III	0	0	12	6
	Discipline Elective	4	0	0	4
	Reading Elective - I	0	0	4	2
Semester Total:		16	0	24	28

Semester - IV

Course Code	Course Name	L	T	P	C*
CHEM 501	Advanced Inorganic Chemistry	4	0	0	4
CHEM 502	Advanced Physical Chemistry	4	0	0	4
CHEM 510	Organic Synthesis	4	0	0	4
CHEM 511	Organotransition - Metal Chemistry	4	0	0	4
CHEM 506L	Chemistry Lab - IV	0	0	12	6
	Open Elective	4	0	0	4
	Reading Elective - II	0	0	4	2
Semester Total:		20	0	16	28

List of Discipline Elective

Course Code	Course Name	L	T	P	C*
CHEM 519	Nanomaterials	4	0	0	4
CHEM 512	Photo - Organic and Heterocyclic Chemistry	4	0	0	4
CHEM 522	Polymer Chemistry	4	0	0	4
ENVS 405	Environmental Chemistry	4	0	0	4

List of Reading Elective

Course Code	Course Name	L	T	P	C*
CHEM 515R	Forensic Science	0	0	4	2
CHEM 517R	Metals in Medicines	0	0	4	2
CHEM 518R	Nano Catalysis	0	0	4	2
CHEM 520R	Pharmaceutical Chemistry	0	0	4	2
BT 604R	Renewable Energy Sources	0	0	4	2
BIO 602R	Bioethics, Biosafety and IPR	0	0	4	2

List of Online Reading Elective

Course Name
ICT in Teaching and Learning

- * **L - Lecture hrs/week; T - Tutorial hrs/week;**
P-Project/Practical/Lab/All other non-classroom academic activities,
etc. hrs/week; C - Credit Points of the Course

Student can opt open (Generic) elective from any discipline of the Vidyapith with prior permission of respective heads and time table permitting.

Every Student shall also opt for:

Five Fold Education: Physical Education I, Physical Education II,

Five Fold Education: Aesthetic Education I, Aesthetic Education II,

Five Fold Education: Practical Education I, Practical Education II

one each semester

Five Fold Activities

Aesthetic Education I/II		Physical Education I/II	
BVFF 101	Classical Dance (Bharatnatyam)	BVFF 201	Aerobics
BVFF 102	Classical Dance (Kathak)	BVFF 202	Archery
BVFF 103	Classical Dance (Manipuri)	BVFF 203	Athletics
BVFF 104	Creative Art	BVFF 204	Badminton
BVFF 105	Folk Dance	BVFF 205	Basketball
BVFF 106	Music-Instrumental (Guitar)	BVFF 206	Cricket
BVFF 107	Music-Instrumental (Orchestra)	BVFF 207	Equestrian
BVFF 108	Music-Instrumental (Sarod)	BVFF 208	Flying - Flight Radio Telephone Operator's Licence (Restricted)
BVFF 109	Music-Instrumental (Sitar)	BVFF 209	Flying - Student Pilot's Licence
BVFF 110	Music-Instrumental (Tabla)	BVFF 229	Aeromodelling
BVFF 111	Music-Instrumental (Violin)	BVFF 210	Football
BVFF 112	Music-Vocal	BVFF 211	Gymnastics
BVFF 113	Theatre	BVFF 212	Handball
Practical Education I/II		BVFF 213	Hockey
BVFF 301	Banasthali Sewa Dal	BVFF 214	Judo
BVFF 302	Extension Programs for Women Empowerment	BVFF 215	Kabaddi
BVFF 303	FM Radio	BVFF 216	Karate - Do
BVFF 304	Informal Education	BVFF 217	Kho-Kho
BVFF 305	National Service Scheme	BVFF 218	Net Ball
BVFF 306	National Cadet Corps	BVFF 219	Rope Mallakhamb
		BVFF 220	Shooting
		BVFF 221	Soft Ball
		BVFF 222	Swimming
		BVFF 223	Table Tennis
		BVFF 224	Tennis
		BVFF 225	Throwball
		BVFF 226	Volleyball
		BVFF 227	Weight Training
		BVFF 228	Yoga

Every Student shall also opt for:

Five Fold Education: Physical Education I, Physical Education II,
 Five Fold Education: Aesthetic Education I, Aesthetic Education II,
 Five Fold Education: Practical Education I, Practical Education II
 one each semester

Evaluation Scheme and Grading System

Continuous Assessment (CA) (Max. Marks)					End-Semester Assessment (ESA) (Max. Marks)	Grand Total (Max. Marks)
Assignment		Periodical Test		Total (CA)		
I	II	I	II			
10	10	10	10	40	60	100

In all theory, laboratory and other non classroom activities (project, dissertation, seminar, etc.), the Continuous and End-semester assessment will be of 40 and 60 marks respectively. However, for Reading Elective, only End semester exam of 100 marks will be held. Wherever desired, the detailed breakup of continuous assessment marks (40), for project, practical, dissertation, seminar, etc shall be announced by respective departments in respective student handouts.

Based on the cumulative performance in the continuous and end-semester assessments, the grade obtained by the student in each course shall be awarded. The classification of grades is as under:

Letter Grade	Grade Point	Narration
O	10	Outstanding
A+	9	Excellent
A	8	Very Good
B+	7	Good
B	6	Above Average
C+	5	Average
C	4	Below Average
D	3	Marginal
E	2	Exposed
NC	0	Not Cleared

Based on the obtained grades, the Semester Grade Point Average shall be computed as under:

$$SGPA = \frac{CC_1 * GP_1 + CC_2 * GP_2 + CC_3 * GP_3 + \dots + CC_n * GP_n}{CC_1 + CC_2 + CC_3 + \dots + CC_n} = \frac{\sum_{i=1}^n CC_i * GP_i}{\sum_{i=1}^n CC_i}$$

Where n is the number of courses (with letter grading) registered in the semester, CC_i are the course credits attached to the i^{th} course with letter grading and GP_i is the letter grade point obtained in the i^{th} course. The courses which are given Non-Letter Grades are not considered in the calculation of SGPA.

The Cumulative Grade Point Average (CGPA) at the end of each semester shall be computed as under:

$$CGPA = \frac{CC_1 * GP_1 + CC_2 * GP_2 + CC_3 * GP_3 + \dots + CC_n * GP_n}{CC_1 + CC_2 + CC_3 + \dots + CC_n} = \frac{\sum_{i=1}^n CC_i * GP_i}{\sum_{i=1}^n CC_i}$$

Where n is the number of all the courses (with letter grading) that a student has taken up to the previous semester.

Student shall be required to maintain a minimum of 4.00 CGPA at the end of each semester. If a student's CGPA remains below 4.00 in two consecutive semesters, then the student will be placed under probation and the case will be referred to Academic Performance Review Committee (APRC) which will decide the course load of the student for successive semester till the student comes out of the probationary clause.

To clear a course of a degree program, a student should obtain letter grade C and above. However, D/E grade in two/one of the courses throughout the UG/PG degree program respectively shall be deemed to have cleared the respective course(s). The excess of two/one D/E course(s) in UG/PG degree program shall become the backlog course(s) and the student will be required to repeat and clear them in successive semester(s) by obtaining grade C or above.

After successfully clearing all the courses of the degree program, the student shall be awarded division as per following table.

Division	CGPA
Distinction	7.50 and above
First Division	6.00 to 7.49
Second Division	5.00 to 5.99
Pass	4.00 to 4.99

CGPA to % Conversion Formula: % of Marks Obtained = CGPA * 10

M. Sc. Chemistry

First Semester

CHEM 401 Analytical Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes

On completion of course, the students will be able to:

- apply knowledge of basic statistics to validate the results of analysis.
- understand various chromatographic techniques and its applications in separation of mixtures, purification of samples, and qualitative and quantitative analysis.
- apply the concept of electrophoresis.
- explain the principle and applications of thermal methods of analysis and atomic spectroscopy

Section-A

Error: types of errors, measurement, accuracy and precision, significant figure, Mean, median and standard deviation,

General introduction to principles and types of chromatography according to shape of chromatographic bed, physical state of mobile phase, mechanism of separation and techniques involved.

Paper Chromatography: Principle, types, choice of paper, visualization, applications.

Thin Layer Chromatography (TLC): Principle, advantage over paper chromatography, types, preparation of thin layer, choice of sorbent and solvent, development, detection and applications.

High Performance Thin Layer Chromatography (HPTLC): Principle, advantage over TLC, instrumentation, choice of sorbent and solvent, development, detection and applications.

Column Chromatography: Principle, column efficiency, factors influencing column efficiency, experimental set up and applications.

Section-B

Gas Chromatography (GC): principle, instrumentation, column efficiency, solvent efficiency, solid supports, liquid phase, liquid phase percentage, column temperature, detectors, chromatographic identification, applications.

High Performance Liquid Chromatography (HPLC): principle, types: partition, adsorption, ion-exchange, size-exclusion or gel; instrumentation,

Ion-Exchange Chromatography: principle, types of ion-exchangers, regeneration, ion-exchange capacity, applications.

Electrophoresis: principle, techniques.

Section-C

Molecular Fluorescence, Phosphorescence and Chemiluminescence:

Principles of luminescence

Instrumentation for fluorescence and phosphorescence, Chemiluminescence, Applications of luminescence techniques

Atomic Absorption Spectroscopy

Principles, Atomization process, Flame atomization, Electrothermal atomization, Atomic line widths and radiation sources for AAS, Instrumentation, Interferences, Background correction methods, Merits, demerits, and applications

Atomic Emission Spectroscopy

Atomic spectra, Population distribution with temperature, Sources: arc, spark and plasma for atomic emission, Spectrometers, Merits, demerits, and applications

Recommended Books

1. Christian, G. D. (2004). *Analytical Chemistry*, 6th Ed., New York: John Wiley.
2. Skoog, D. A., West, D. M., Hollar, F. J. & Crouch S. R. (2014). *Fundamentals of Analytical Chemistry*, 9th Ed., U.S.: Cengage Limited.
3. Willard, H. L., Merritt, L., Dean, J.A. & Settle, F.A. (2004). *Instrumental Methods of Analysis*, 7th Ed., India: CBS Publishing.
4. Ewing, G.W. (1985). *Instrumental Methods of Chemical Analysis*, 5th Ed., U.S.: McGraw-Hill College.

- Holler, F.J., Skoog, D. A. & Crouch, S. R. (2007). *Principles of Instrumental Analysis*, 6th Ed., New York: Belmont, CA: Thomson Brooks/Cole.
- Mendham, J., Denney, R.C., Barnes, J.D. & Thomas, M. (2000). *Text Book of Quantitative Inorganic Analysis*, 6th Ed., U.S.: Prentice Hall

Suggested e-Sources

- National programme on technology enhanced learning
<https://nptel.ac.in>
- Online chemistry courses
<https://www.edx.org/learn/chemistry>
- Free online education swayam
<https://swayam.gov.in>

CHEM 405 Inorganic Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- appreciate the role of molecular orbital theory in explaining geometry of molecules.
- analyze the bonding and structural aspects of chemical species of main group elements.
- explain the mechanistic aspects of metal complex reactions and relate it to the stability of metal complexes.
- determine the symmetry operations of molecules.
- apply group theory to study the hybridization and vibrational modes of molecules.

Section-A

Structure, Reactivity and Bonding:

- (a) **Structure and Reactivity of Main Group Elements:** VSEPR, Walsh diagrams (AB_2 and AB_3 molecules e.g. H_2O and BH_3), $d\pi-p\pi$ bonds,

Bent's and energetics of hybridization, some simple reaction of covalently bonded molecules.

- (b) Bonding in Metal Complexes:** Molecular orbital theory: octahedral, tetrahedral and square planar complexes, π bonding, η^2 , η^3 , η^5 , η^6 systems with reference to molecular orbital theory.

Section-B

Reaction Mechanism of Transition Metal Complexes:

Energy profile of a reaction, reactivity of metal complexes, inert and labile complexes, kinetic and thermodynamic stability of metal complexes, kinetics of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal-ligand bond cleavage, substitution reactions in square planar complexes, the trans effect, mechanism of the substitution reactions, redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Section-C

Symmetry and Group Theory in Chemistry:

Symmetry operations, symmetry elements, group, subgroup, relation between order of a finite group and its subgroup, similarity transformation and classes, molecular point groups and their classification, representations of groups by matrices (representation for the C_n , C_{nv} and D_{nh} only), characters and properties of representation, relationship between reducible and irreducible representations, great orthogonality theorem, character table (C_{2v} and C_{3v} only).

Applications of Group Theory in Chemistry:

Formation of hybrid orbitals: σ -bonding in trigonal planar (BF_3), tetrahedral (CH_4), square pyramidal (BrF_5) and square planar (XeF_4), prediction of infrared and Raman active vibrational modes in H_2O and BF_3 molecules

Ligand Field Theory: Splitting of levels and terms in a chemical environment, energy level diagrams and construction of energy level diagrams.

Recommended Books

1. Bhattacharya, P., *Group theory and its chemical applications*. India: Himalaya Prakashan.
2. Cotton, F.A., *Group theory and its chemical applications*. New York : Wiley.
3. Cotton F.A., Wilkinson G., Murillo C.A., Bochmann M. (1999). *Advanced Inorganic Chemistry, 6th Ed.*, New York : John Wiley & Sons.
4. Huheey J.E., Harpes, Row. (1997). *Inorganic chemistry, Principles of Structure and Reactivity, 4th Ed.*, India: Pearson Publications.
5. Greenwood N.N., Earnshaw A. (1997), *Chemistry of the element, 2nd Ed.*, Amsterdam, Netherlands : Elsevier.
6. Carlin R.L., (1986). *Magnetochemistry*, New York : Springer Verlag.
7. McCleverty J.A., Meyer T.J. (2003). *Comprehensive coordination chemistry II, 2nd Ed.*, Amsterdam, Netherlands : Elsevier.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 406 Organic Chemistry**Max. Marks : 100****L T P C****(CA: 40 + ESA: 60)****4 0 0 4****Learning Outcomes:**

On completion of course, the students will be able to:

- understand the concept of aromaticity, nonaromaticity and antiaromaticity in organic compounds.

- explain the reaction mechanism, preparation, reactivity and stability of reaction intermediates.
- understand and apply the concepts of stereochemistry.
- explain the aliphatic nucleophilic substitution reactions.

Section-A

Aromaticity:

Huckel's MO (HMO) theory, PMO theory, aromaticity in benzenoid and non-benzenoid compounds: Huckel's rules, aromatic, anti-aromatic, homo-aromatic compounds; alternant and non-alternant hydrocarbons; fullerenes.

Addition compounds:

Crown ethers, phase transfer catalysis, ionic liquids, inclusion compounds and cyclodextrins.

Reaction Mechanism and its Determination:

Types of mechanism, potential energy diagram, transition states and intermediates, methods of determining mechanisms (product analysis, intermediates analysis, isotope effect, kinetic and stereochemical studies).

Reactive Intermediates:

Generation, structure, stability and reactivity of carbocation, carbanion, free radical, carbene, nitrene and aryne.

Section-B

Stereochemistry:

Conformational analysis of decalins, effects of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding, threo and erythro isomers, enantiotopic and diastereotopic atoms, groups faces, stereospecific and stereoselective synthesis, asymmetric synthesis (chiral pool and chiral auxiliaries), optical activity in the absence of chiral carbon (biphenyl, allenes and spirans).

Section-C

Aliphatic Nucleophilic Substitution:

The S_N2 , S_N1 , mixed S_N1 and S_N2 , S_N^i and SET mechanisms; effects of substrate structure, attacking nucleophile, leaving group and reaction medium on the types of mechanism; nucleophilic substitution at an allylic,

aliphatic trigonal and a vinylic carbon atom; neighbouring group participation by π - and σ -bonds, classical and non-classical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements: acid catalysed rearrangement of carbonyl compounds, rearrangement of epoxides, transannular rearrangement, rearrangement of camphene hydrochloride to isobornyl chloride; ambident nucleophile, regioselectivity.

Recommended Books

1. Smith M. B., March J. (2007). *March's Advanced Organic Chemistry Reaction Mechanism and Structure. (6th ed.)*. New York : John Wiley & Sons.
2. Carey, F. A., Sundberg, R. J. (2007). *Part A: Structure and Mechanism. (5th ed.)*. Berlin, Germany: Springer.
3. House, H. O., Benjamin, W. A. (1965). *Modern Organic Reactions*. Publisher: New York.
4. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2001). *Organic chemistry. (2nd ed.)*. Publisher: Oxford University Press.
5. Sykes, P. (1986). *A guide book to mechanism in organic chemistry (6th ed.)*. Singapore: Pearson Education Pvt. Ltd.
6. Ingold, C. K. (1970). *Structure and mechanism in organic chemistry*. New York : Cornell University Press.
7. Morrison, R.T., Boyd, R.N. (2002). *Organic chemistry (6th Ed.)*. Prentice Hall: Englewood Cliffs, NJ.
8. Nasipuri, D. (1994). *Stereochemistry of organic compounds. (2nd ed.)*. India: New Age International.
9. Singh, M.S. (2005). *Advanced organic chemistry-reactions and mechanisms*. Singapore: Pearson Education Pvt. Ltd.
10. Wade, L.G., Singh, M.S. (2008). *Organic chemistry*. Singapore: Pearson Education, (Dorling Kindersley Pvt. Ltd.
11. Singh, M.S. (2014). *Reactive intermediates in organic chemistry-structure, mechanism and reactions*. Germany: Wiley, VCH, & Weinheim.
12. Eliel E. L., Wilen S. H., Manden L. N. (2005). *Stereochemistry of Carbon compounds*. New York : Wiley & sons.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 408 Physical Chemistry**Max. Marks : 100****L T P C****(CA: 40 + ESA: 60)****4 0 0 4****Learning Outcomes:**

On completion of course, the students will be able to:

- calculate the energy of one dimensional, three dimensional box, harmonic oscillator, rigid rotor and hydrogen atom, and explain the variation and perturbation theory and its application for hydrogen atom.
- apply the concept of nuclear reactions and calculate the fission product yield.
- understand the radioactive techniques: neutron activation analysis, GM counter, ionization counter and tracer techniques.
- derive the relationship between thermodynamic equations and solve the numerical problems.
- explain the collision theory, activated complex theory and Lindemann's theory of reaction rates.

Section-A**Quantum Chemistry:**

Introduction quantum mechanics, Schrodinger equation and the postulates of quantum mechanics, discussion of solutions of the Schrodinger equation to some model systems viz. particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom.

Approximate Methods:

The variation theorem, linear variation principle Perturbation theory (first order and non-degenerate), and applications of variation method and perturbation theory to the hydrogen atom.

Section-B**Thermodynamics:**

Partial molar properties, partial molar free energy, partial molar volume and partial molar heat constant and their significance, determination of these quantities, chemical potential and its variation with temperature and pressure, degree of advancement of reaction, de Donder's treatment of chemical equilibria, variation of equilibrium constant with temperature and pressure, Le Chatelier principle and its thermodynamic derivation, fugacity of gases and mixture of ideal and real gases, determination of fugacity and its variation with temperature and pressure, thermodynamic functions of mixing, ideal solutions and Raoult's laws, Henry's law, solubility behavior of ideal solutions.

Section-C**Chemical Dynamics:**

Collision theory of reaction rates, steric factors, activated complex theory, Arrhenius equation and activated complex theory, reactions in solution ion and ion-dipole interactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions (Lindman's theory), homogeneous catalysis and kinetics of enzyme catalysis.

Nuclear and Radiochemistry:

Nuclear structure and nuclear stability, radioactive decay and equilibrium, nuclear reactions, Q-value, cross sections, types of reactions (nuclear fission and fusion), fission products and yields, radioactive techniques, tracer technique, neutron activation analysis, counting techniques: GM, ionization counter.

Recommended Books

1. Atkin's, P., Julio, P. D., (2014). *Physical Chemistry* (10th ed.), U. K., Oxford University Press.

2. Castellan, G.W., (1983). *Physical Chemistry* (3rd ed.), USA, Addison-Wesley Publishing Company.
3. Chandra, A. K., (2006). *Introduction to Quantum Chemistry* (4th ed.), India, Tata McGraw Hill Publishing Company Ltd.
4. Levine, I. N., (2014). *Quantum Chemistry* (7th ed.), USA, Pearson Education.
5. Laidler, K.J., (1965) *Chemical Kinetics* (2nd ed.), New York, McGraw Hill Book Company.
6. Rajaraman, J., Kuriacose, J. C., (1993). *Kinetics and Mechanism of Chemical Transformations*, India, Macmillan Publishers India Limited.
7. Arniker, H. J. (2005). *Essentials of Nuclear Chemistry* (4th ed.), India, New Age International Ltd. Publisher.
8. Puri, B.R., Sharma, L.R., Pathania, M.S. (2016). *Principle of Physical Chemistry* (47th ed.), India, Vishal Publishing Company.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
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2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

MATH 407 Mathematics for Chemists

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- Use matrices techniques for solving system simultaneous linear equations.
- Apply elementary transformations to reduce the matrix to Echelon and normal form and determine its rank.

- Solve differential equation problems in the field of Chemistry.
- Demonstrate knowledge of probability and some basic statistical measures.

Section-A

Logarithms:

Definition, laws regarding product, quotient, power and change of base, the logarithmic and exponential series.

Matrix Algebra:

Definition, types of matrices, matrix addition and multiplication with their properties, determinants (examples from Huckel theory), and their properties (without proof), transpose, adjoint and inverse of matrices, special matrices (symmetric, skew-symmetric, Hermitian, skew-Hermitian, orthogonal and unitary) and their properties, homogenous, non-homogenous linear equations, conditions of consistency and solution by Cramer's rule, inverse matrix method and matrix method, linear dependence and independence, Eigen values and Eigen vectors, diagonalization.

Section-B

Differential Calculus:

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

Integral calculus:

Integration as inverse operation of differentiation, methods of integration-integration by parts, integration by substitution and by partial fraction

Section-C

Ordinary Differential Equation:

Solution of differential equations of first order and first degree when equation is in variable separable form, homogeneous, linear and exact, applications to chemical kinetics, regular equilibria, quantum chemistry,

spherical harmonics, second order, differential equation with constant coefficients and their solutions.

Permutation and Probability:

Permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors examples from the kinetic theory of gases, curve fitting (including least squares fit) with a general polynomial fit.

Recommended Books

1. Singh, B. (2010). *Mathematics for Chemists*, India, Pragti Prakashan.
2. Sharma, G. C., Jain, M. (2001). *Essential Mathematics*, India, Galgotia Publication.
3. Tebbutt, P. (1998). *Basic Mathematics for Chemists*, Wiley.
4. Barrante, J. R. (2004). *Applied Mathematics for Physical Chemistry* (3rd ed.), Pearson Prentice Hall.
5. Daniels, F., (1928). *Mathematical Preparation for Physical Chemistry*, McGraw Hill.
6. Hirst, D. M., *Chemical Mathematics*, Longman.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 402L Chemistry Lab-I

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

0 0 12 6

Learning Outcomes:

On completion of course, the students will be able to:

- develop their skills for qualitative and quantitative research in different fields
- perform various analytical operations to qualify and quantify different organic and inorganic samples
- present information and write reports in a clear, effective and scientific manner

Inorganic Chemistry

Qualitative and Quantitative Analysis:

1. Qualitative analysis of mixture of salts (soluble and insoluble) containing six radicals including one less common metal ions-Tl, Mo, W, Se, Ti, Zr, Th, Ce, V and U.
2. Separation and determination of two metal ions Cu-Ni, Ni-Zn, Cu-Fe etc. involving volumetric and gravimetric methods.

Organic Chemistry

Qualitative Analysis:

1. Analysis of binary mixture using NaHCO_3 , NaOH , H_2O , HCl and organic solvent and preparation of suitable derivatives.
2. Separation of following binary organic mixture by column chromatography and preparative TLC:
 - (a). *o*-bromo and *p*-bromo aniline
 - (b). *o*-bromo and *p*-bromo acetanilide
 - (c). *o*-nitro and *p*-nitro aniline
 - (d). *o*-nitro and *p*-nitro phenol

One-step Organic Synthesis:

1. Reduction: Synthesis of benzhydrol from benzophenone.
2. Oxidation: Synthesis of *p*-chlorobenzoic acid from *p*-chlorotoluene.

3. Aldol condensation: Synthesis dibenzalacetone from benzaldehyde.
4. Cannizzaro reaction: 4-chlorobenzaldehyde as substrate.

Physical Chemistry

Error Analysis and Statistical Data Analysis:

Errors, types of errors, minimization of errors, error distribution curves, precision, accuracy and combination; statistical treatment for error analysis, students' t' test, null hypothesis, rejection, criteria, F & Q test, linear regression analysis, curve fitting.

Partition Coefficient

1. To find out partition coefficient of iodine between CCl_4 and H_2O .
2. To find out the partition coefficient of benzoic acid between C_6H_6 and water.

Phase Equilibria

1. Determination of congruent composition and temperature of a binary system (diphenylamine-benzophenone system).
2. Determination of glass transition temperature of a given salt (CaCl_2) conductometrically.
3. To construct the phase diagram for three component system (chloroform-acetic acid-water).

Chemical Kinetics

1. Determination of the effect of (a) change of temperature (b) change of concentration of reactants and catalysts and (c) ionic strength of the media on the velocity constant of hydrolysis of an ester/ionic reactions.
2. Determination of the velocity constant of hydrolysis of an ester/ionic reaction in micellar media.
3. Determination of the rate constant for the oxidation of iodide ions by hydrogen peroxide studying the kinetics as an iodine clock reaction.
4. Flowing clock reactions (Ref: experiments in physical chemistry by Showmaker).
5. Determination of the primary salt effect in the kinetics of ionic reactions and testing of the Bronsted relationship (iodide ion is oxidized by persulphate ion).

6. To find out the order of reaction between potassium bromate and potassium iodide.

Recommended Books

1. Gurdeep, R. (2016). *Advanced Practical Inorganic Chemistry*, Revised Ed., India: Krishna Prakashan Publication.
2. Svehla, G. (2010). *Vogel's Qualitative Inorganic Analysis*, 5th Ed., U.S.: Prentice Hall.
3. Gurtu, J. N. & Gurtu, A. (2011). *Physical Chemistry Vol. I*, India: Pragati Prakashan Publication.
4. Leonard, J., Lygo, B. & Procter, G. (2013). *Advanced Practical Organic Chemistry*, 3th Ed., U.K.: CRC Press, Taylor & Francis Group.
5. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. (1989). *Practical Organic Chemistry*, 5th Ed., New York: John Wiley & Sons, Inc.
6. Gurtu, G.N., Gurtu, A. (2014). *Advanced Physical Chemistry*, India: Pragati Prakashan Publication.
7. Sindhu, P.S. (2005). *Practicals in Physical Chemistry*, India: Macmillan Publishers.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
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3. Free Online Education SWAYAM
<https://swayam.gov.in>

Second Semester

CHEM 412 Special Topics in Physical Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- understand the principles and theory of corrosion
- understand the mechanism and kinetics of corrosion
- calculate the surface area of adsorbents
- calculate molecular mass of polymers
- understand the various theory of magnetism and differentiate material on the basis of theory

Section-A

Corrosion:

Scope and economics of corrosion, causes and types of corrosion: Dry corrosion, electrochemical theories of corrosion, Galvanic cell corrosion and Pitting corrosion. Kinetics of corrosion: corrosion current and corrosion potential. Corrosion measurements: weight loss, OCP measurement, and linear polarization resistance methods. Corrosion prevention: electrochemical, inhibitor, and protective metallic coatings.

Kinetics of Electrode Reactions:

Theoretical investigation of kinetics of an Electrode reactions, Diffusion over potential, instrumentation, current-potential relation applicable for Linear Sweep Voltammetry (LSV) and Cyclic Voltammetry (CV), interpretation of cyclic voltammograms and parameters obtainable from voltammograms.

Section-B

Surface Chemistry:

Surface tension, capillary action, pressure difference across curved surface (Laplace equation), vapor pressure of droplets (Kelvin equation), Gibbs adsorption isotherm, BET theory, mathematical derivation of BET equation, estimation of surface area using BET equation, surface films on liquids (Electro-kinetic phenomenon).

Polymer:

Polymer: definition, types of polymers, kinetics of polymerization, mechanism of polymerization, molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry and diffusion), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

Section-C

Magneto Chemistry:

Magnetic susceptibility and its determination, susceptibility equivalents, Pascal's law and its applications, diamagnetism of elements, compounds and ions, Langevin's theory of paramagnetism, Curie's law, Weiss molecular field theory of paramagnetism, Curie-Weiss law, determination of Curie point.

Chemical Bonding: Molecular Quantum Mechanics;

Elementary concepts of MOT for homonuclear diatomic molecules, VBT theory, Huckel theory of conjugated systems, bond order and charge density, calculations, applications on ethylene, butadiene, cyclopropenyl radical, cyclobutadiene and benzene; introduction to extended Huckel theory.

Recommended Books

- 1 Laider, K.J., (1965) *Chemical Kinetics* (2nd ed.), New York, McGraw Hill Book Company.
- 2 Gowariker, V.R., Vishwanathan, N.V., & Sridhar, J., (1986) *Introduction to polymer science*, New York, John Wiley & Sons.
- 3 Atkin's, P., Julio, P. D., (2014). *Physical Chemistry* (10th ed.), U. K., Oxford University Press.

- 4 Selwood, P.W., (2013). *Magneto chemistry*, Swin burne Press.
- 5 Chandra, A. K., (2006). *Introduction to Quantum Chemistry* (4th ed.), India, Tata McGraw Hill Publishing Company Ltd.
- 6 Levine, I. N., (2014). *Quantum Chemistry* (7th ed.), USA, Pearson Education.
- 7 Puri, B.R., Sharma, L.R., Pathania, M.S. (2016). *Principle of Physical Chemistry* (47th ed.), India, Vishal Publishing Company.
- 8 Gabor, A., Somorjai, Yimin L. (2010) *Introduction to Surface Chemistry & Catalysis*, New York, John Wiley & Sons.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
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3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 407 Organic Reaction Mechanism

Max. Marks : 100	L T P C
(CA: 40 + ESA: 60)	4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- understand the aromatic electrophilic and nucleophilic substitution reactions, and free radical reactions.
- explain the addition to C-C and C-X multiple bonds, and elimination reactions.
- understand the pericyclic reactions.

Section-A

Aromatic Electrophilic Substitution:

The arenium ion mechanism, orientation and reactivity, energy profile diagrams, the ortho/para ratio, ipso attack, diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction.

Aromatic Nucleophilic Substitution:

The S_NAr , benzyne and $S_{RN}1$ mechanisms, reactivity effect of substrate structure, leaving group and attacking nucleophile, Von-Richter, Sommelet-Hauser and Smiles rearrangements.

Free Radical Reactions:

Types of free radical reactions, free radical substitution mechanism, allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts, Sandmeyer reaction, free radical rearrangements, Hunsdiecker reaction.

Section-B

Addition to Carbon-Carbon Multiple Bonds:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals; regio and chemoselectivity, orientation and reactivity, hydroboration, Michael reaction, Sharpless asymmetric epoxidation.

Addition to Carbon-Hetero atom Multiple Bonds:

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

Elimination Reactions:

The E^1 , E^2 and E^1cB mechanisms, orientation of the double bond, reactivity effect of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Section-C

Pericyclic Reactions:

Introduction, classification of pericyclic reactions, frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allylic systems; molecular orbital symmetry: m -plane and C_2 -axis, molecular orbitals of polyene systems, analysis of pericyclic reactions:- correlation diagram, FMO method and PMO approach; electrocyclic reactions:- conrotatory and disrotatory motions, $4n$ and $4n+2$ π -systems; cycloadditions:- classification, antarafacial and suprafacial additions, $2\pi + 2\pi$ and $4\pi + 2\pi$ addition, $2\pi + 2\pi$ addition of ketenes; sigmatropic rearrangements:- suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5-sigmatropic rearrangements, Claisen and Cope rearrangements.

Recommended Books

1. Smith, M. B., March, J. (2007). *Advanced Organic Chemistry Reaction Mechanism and Structure*. 6th ed.). A John Wiley & Sons (
2. Carey, F. A., Sundberg, R. J. (2007). *Part A : Structure and Mechanism*. (5th ed.). Springer
3. House, H. O., Benjamin, W. A. (1965). *Modern Organic Reactions*. W.A Benjamin New York.
4. Clayden, J., Greeves, N., Warren, S., Wothers, P. (2001). *Organic chemistry*. (2nd ed.). Oxford University Press.
5. Sykes, P. (1986). *A guide book to mechanism in organic chemistry* (6th ed.). Pearson.
6. Ingold, C. K. (1970). *Structure and mechanism in organic chemistry*. Cornell University Press.
7. Morrison, R.T., Boyd, R.N. (2002). *Organic chemistry* (6th Ed.). PrenticeHall: Englewood Cliffs, NJ.
8. Nasipuri, D. (1994). *Stereochemistry of organic compounds*. (2nd ed.). New Age International
9. Singh, M.S. (2005). *Advanced organic chemistry-reactions and mechanisms*. Pearson Education (Singapore) Pvt. Ltd.
10. Wade, L.G., Singh, M.S. (2008). *Organic chemistry*. Pearson Education, (Dorling Kindersley Pvt. Ltd.

11. Singh, M.S.(2014). *Reactive intermediates in organic chemistry- structure, mechanism and reactions*. Wiley, VCH, & Weinheim.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 411 Photo Inorganic Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- understand the basic and fundamental concepts involved in photochemistry.
- explain the physical and photochemical processes for the excitation of molecules using Jablonski diagram.
- understand the optical properties, optical rotatory dispersion and its applications.
- explain the types and mechanism of photochemical reactions of transition metal complexes.
- describe the charge transfer transitions in transition metal complexes.

Section-A

Photochemistry:

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, internal conversion and intersystem crossing, quantum yield, photosensitized reactions, energy transfer process (simple examples).

Optical Rotation and Circular Dichroism:

Principles and fundamentals, optically active molecules, optically rotatory dispersion, circular dichroism, relationship between optically rotatory dispersion and circular dichroism curves and their use in coordination chemistry

Section-B

Photochemistry of Carbonyl Complexes:

Introduction, $\text{Cr}(\text{CO})_6$, $\text{Fe}(\text{CO})_5$ and $\text{Ni}(\text{CO})_4$.

Photosubstitution Reactions:

Introduction, photosubstitution of d^3 , low spin d^6 and d^8 complexes, sensitization and quenching of photosubstitution, photosubstitution mechanism, photoisomerisation, photoracemization and photoanation..

Section-C

Redox Reactions by Excited Metal Complexes:

Charge transfer spectra, ligand to metal charge transfer, metal to ligand charge transfer, intraligand and charge transfer to solvent state, metal complexes as redox reactants, reducing and oxidizing properties of $\text{Ru}(\text{bipy})_3$, comparison with $\text{Fe}(\text{bipy})_3$, role of spin-orbit coupling, applications of redox processes of low energy reactants into high-energy products and chemical energy into light.

Recommended Books

1. Basolo, F., & Pearson, R. (1967). *Mechanism of organic reaction: a study of metal complexes in solution*, (2nd ed.): John Wiley & Sons.
2. Obe, M.L. (1972). *Inorganic reaction mechanism*: Nelson, London.
3. Purcell, K.F., & Kotz, J.C. (1980) *An introduction to inorganic chemistry*: Holt Sounder, Japan.
4. Adamson, A.W., & Fleischauer, P.D. (1977) *Concepts of inorganic photochemistry*: Wiley.
5. Porter, G.B. (1983). *Introduction to inorganic photochemistry: Principles and methods*: *J. Chem. Educ.* 60(10), p 785.

- Balzari, V., & Carassiti, V. (1970). *Photochemistry of coordination compounds*: Academic Press.
- Ferraudi, G.J. (1988). *Elements of inorganic photochemistry*: Wiley.

Suggested e-Sources

- National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
- Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
- Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 409 Spectral Techniques in Inorganic Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- explain the rules for predicting molecular structure of metal complexes with the help of electronic spectral study.
- apply the knowledge of heteronuclear magnetic resonance spectroscopy for characterization of inorganic compounds.
- characterize some iron and tin complexes with the help of Mössbauer spectroscopy.
- explain the bonding and structures of paramagnetic metal complexes using ESR spectroscopy.
- characterize inorganic compounds which have quadruple nucleus with the help of nuclear quadrupole resonance spectroscopy.

Section-A

Electronic Spectroscopy:

Spectroscopic ground states, Orgel and Tanabe-Sugano diagrams for transition metal complexes (d^1 - d^9 states); spectrochemical series, calculations of Dq , B and β parameters, charge transfer spectra,

spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information, anomalous magnetic moments, magnetic exchange coupling and spin crossover, structural evidence from electronic spectra.

Section-B

Nuclear Magnetic Resonance (NMR) Spectroscopy:

Application of chemical shifts, signal intensities and spin-spin coupling to structure determination of inorganic compounds carrying NMR active nuclei like ^1H , ^{11}B , ^{15}N , ^{19}F , ^{29}Si , ^{31}P , effect of fast chemical reactions, coupling to quadrupolar nuclei, NMR of paramagnetic substances in solution, nuclear and electron relaxation time, contact shift, pseudo-contact shift, factoring contact and pseudo-contact shift for transition metal ions, contact shift and spin density, π -electron delocalization, application to planar tetrahedral equilibrium, contrast agents.

Mossbauer Spectroscopy:

Doppler shift and recoil energy, isomer shift and its interpretation, quadrupole interactions, effect of magnetic field on Mossbauer spectra, applications to metal complexes, metal carbonyls, Fe-S cluster and tin compounds.

Section-C

Electronic Paramagnetic Resonance (EPR) Spectroscopy: Electronic Zeeman effect and EPR transition energy, EPR spectrometers, presentation of spectra. effects of electron Zeeman, Hyperfine splittings in isotropic systems, spin polarization mechanism and McConnell's relations Anisotropy in g-value, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes.

Nuclear Quadrupolar Resonance (NQR) Spectroscopy: Quadrupolar moment, energy levels of a quadrupolar nucleus and effect of asymmetry parameters and energy levels, Effect of an external magnetic field, selected examples for elucidation of structural aspects of inorganic compounds using NQR spectroscopy.

Recommended Books

1. Lever, A.B.P. (1984). *Inorganic Electronic Spectroscopy*, Amsterdam: Elsevier

2. Ebsworth, E. A.O. (1991). *Structural Methods in Inorganic Chemistry*, Denmark: Blackwell Scientific Publications.
3. Drago, R. S. (1977). *Physical Methods in Chemistry*, U.K.: WB Saunders Co.
4. Carrington, A. & McLachlan, A. D. (1983). *Introduction to Magnetic Resonance*, New York: Chapman & Hall.
5. Parish, R.V. (1991). *NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry*, 1st Ed., U.S.: Ellis Hardwood Ltd.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 410 Spectroscopy

Max. Marks : 100

(CA: 40 + ESA: 60)

L T P C

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- explain the principle and instrumentation of UV-visible, IR, NMR and mass spectroscopy.
- elucidate the structures of compounds using UV-visible, IR, NMR and mass spectral data.
- understand the reaction mechanisms using NMR and mass spectral data.
- characterize the chemical species using UV-visible and IR spectral data.

Section-A

Fundamentals of Spectroscopy:

Electromagnetic radiation, Born-Oppenheimer approximation, types of spectra, intensity of spectral lines, transition probability, natural line width and natural line broadening, selection rules.

UV Spectroscopy:

Principles of absorption spectroscopy, nature of electronic excitations, the origin of UV bands, chromophores, auxochromes, factors affecting the position of UV bands, calculation of λ_{\max} , qualitative and quantitative applications.

Infrared Spectroscopy:

Modes of vibration, vibrations of polyatomic molecules, Principle, the Hook's law and calculation of frequencies for different types of bonds, Instrumentation, sample handling, anharmonicity, overtones, combination bands, Fermi resonance, group frequencies, factors affecting the band positions and intensities, applications.

Section-B

One-dimensional Nuclear Magnetic Resonance Spectroscopy:

Nuclear spin, nuclear resonance, basic, equivalent and non-equivalent protons, shielding and deshielding of nuclei, chemical shift and its measurements, factors influencing chemical shifts, instrumentation of NMR, spin-spin interactions, factors influencing coupling constant 'J', classification of spectra, types of spin systems (AX, ABX, AMX, ABC, A₂B₂, AA'MM'X etc.), shift reagents, spin decoupling, protons on oxygen, nitrogen and sulphur (proton exchange), nuclear overhauser effect, applications of NMR spectroscopy.

Two-dimensional Nuclear Magnetic Resonance Spectroscopy:

Introduction, pulse sequence, 2D-experiments, data collection, processing and plotting of 2D spectra, general procedure for running 2D spectra, COSY, DQF-COSY, TOCSY, NOESY, ROESY, INADEQUATE, HETCOR, HSQC, HMQC, HMBC.

Section-C

¹³C NMR Spectroscopy:

Carbon-13 nucleus, chemical shifts and their calculation, spin-spin coupling with ^1H , ^{13}C , cross-polarization, nuclear overhauser effect, DEPT.

Mass Spectrometry:

Basic principles, production of ions by electron impact, chemical ionization and field desorption techniques, separation and detection of ions, mass spectrum, empirical rules for fragmentation of organic molecules, identification of molecular ion peaks, base peaks, metastable peaks and isotopic peaks, determination of molecular weight and molecular formula of compounds, nitrogen rule, hydrogen deficiency index; introduction to GCMS, LCMS and HRMS.

Structure Elucidation:

Combined structure elucidation problems based on UV, IR, NMR and MS spectrum data to find out the structure of simple organic compounds.

Recommended Books

1. Pavia, D. L., Lampman, G. M. & Kriz, G. S. (2009). *Introduction to Spectroscopy*, (4th ed.): Thomson Learning.
2. Kemp, W. (1991). *Organic Spectroscopy*, (3rd ed.): Palgrave Houndmills. Basingstoke, Hampshire RG21 6XS and 175 Fifth Avenue. New York.
3. Mohan, J. (2001). *Organic Spectroscopy: Principles and Applications*, India: Narosa Publication, New Delhi.
4. Kalsi, P. S. (2016). *Organic Spectroscopy*. (7th ed.), India: New Age International Publishers, New Delhi
5. Silverstein, R. M., Webster, F. X., & Kiemle, D., (2005). *Spectrometric Identification of Organic Compounds*, (7th ed.): John Wiley & Sons.
6. Hoffmann, E. D., & Stroobant, V., (2007). *Mass Spectrometry: Principles and Applications*, (3rd ed.): John Wiley & Sons.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
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2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM

<https://swayam.gov.in>

CHEM 403L Chemistry Lab-II

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

0 0 12 6

Learning Outcomes:

On completion of course, the students will be able to:

- develop their skills for qualitative and quantitative research in different fields.
- perform various analytical operations to qualify and quantify different analytes.
- outline synthetic strategies for important chemicals.
- check the purity of synthesized compounds through TLC, conductance and magnetic susceptibility measurements, and UV, FT-IR spectral data

Inorganic Chemistry

Preparation, purification and structural studies (magnetic, electronic and IR) of inorganic complex compounds:

- (i) trans-potassium diaquabis (oxalato) chromate (III), trans- $K[Cr(ox)_2(H_2O)_2]$
- (ii) vanadyl bis (acetylacetonate) $[VO(acac)_2]$.
- (iii) sodiumdiamminetetraithiocyanatochromate(III), $Na[Cr(NH_3)_2(SCN)_4]$
- (iv) bis(acetate)chromate(II), $[Cr(OAc)_2] \cdot 2H_2O$.
- (v) cis-potassium diaquabis(oxalato)chromate(III), cis- $K[Cr(ox)_2(H_2O)_2]$
- (vi) tris(acetylacetonato)manganese(III), $[Mn(acac)_3]$
- (vii) potassium trioxalatoferrate(III) trihydrate, $K_3[Fe(C_2O_4)_3] \cdot 3H_2O$.
- (viii) Prussian blue, $Fe_3[Fe(CN)_6]_3$.
- (ix) sodium hexanitritocobaltate(III), $Na_3[Co(ONO)_6]$.
- (x) pentaamminemonochlorocobalt(III) chloride, $[CoCl(NH_3)_5]Cl_2$.

- (xi) pentaammineaquacobalt(III) chloride, $[\text{Co}(\text{H}_2\text{O})(\text{NH}_3)_5]\text{Cl}_3$ by using $[\text{CoCl}(\text{NH}_3)_5]\text{Cl}_2$ as the starting material.
- (xii) pentaamminenitritocobalt(III) chloride, $[\text{Co}(\text{ONO})(\text{NH}_3)_5]\text{Cl}_2$ by using $[\text{CoCl}(\text{NH}_3)_5]\text{Cl}_2$ as the starting material.
- (xiii) pentaamminenitrocobalt(III) chloride, $[\text{Co}(\text{NO}_2)(\text{NH}_3)_5]\text{Cl}_3$ by using $[\text{CoCl}(\text{NH}_3)_5]\text{Cl}_2$ as the starting material.

Green Methods of Preparation

- (i). bis(acetylacetonato)copper(II)
- (ii). tris(acetylacetonato)iron(III)
- (iii). tris(acetylacetonato)manganese(III)

Organic Chemistry

Quantitative Analysis

- (i). Determination of the percentage of number of hydroxyl groups in an organic compound by acetylation method
- (ii). Estimation of amines/phenols using bromate-bromide solution or acetylation method
- (iii). Determination of iodine and saponification values of an oil sample
- (iv). Determination of DO, COD and BOD of water sample.

Two-Steps Organic Synthesis

- (i). Anthranilic acid from phthalic anhydride (Phthalic anhydride \rightarrow Phthalimide \rightarrow Anthranilic acid).
- (ii). Hydroquinone to 2,5-dihydroxyacetophenone (Hydroquinone \rightarrow Hydroquinone diacetate \rightarrow 2,5-dihydroxyacetophenone).
- (iii). 2,4-dinitrophenylhydrazine from Chlorobenzene (Chlorobenzene \rightarrow 2,4-dinitrochlorobenzene \rightarrow 2,4-dinitrophenylhydrazine).
- (iv). Anthroquinone from phthalic anhydride (phthalic anhydride \rightarrow *o*-benzoyl benzoic acid \rightarrow Anthroquinone).
- (v). Acridone from *o*-chlorobenzoic acid (*o*-chlorobenzoic acid \rightarrow *N*-Phenylanthanilic acid \rightarrow Acridone)

Physical Chemistry

Solutions:

- (i). Determination of molecular weight of non-volatile and non-electrolyte/electrolyte by cryoscopic method and to determine the activity coefficient of an electrolyte.
- (ii). Determination of the degree of dissociation of weak electrolyte and to study the deviation from ideal behavior that occurs with a strong electrolyte.

Electrochemistry**A. Conductometry:**

- (i). Determination of the velocity constant, order of the reaction and energy of activation for saponification of ethyl acetate by sodium hydroxide conductometrically
- (ii). Determination of solubility and solubility product of sparingly soluble salts (e.g. PbSO_4 , BaSO_4) conductometrically.
- (iii). Determination of the strength of strong and weak acids in a given mixture conductometrically.
- (iv). To study the effect of solvent on the conductance of AgNO_3 /acetic acid and to determine the degree of dissociation and equilibrium constant in different solvents and in their mixtures (DMSO, DMF, dioxane, acetone and water) and to test the validity of Debye-Huckel-Onsager theory.
- (v). Determination of the activity coefficient of zinc ions in the solution of 0.002M zinc sulphate using Debye-Huckel's limiting law.

B. Potentiometry/pH metry:

- (i). Determination of strength of halides in a mixture potentiometrically.
- (ii). Determination of the valency of mercurous ions potentiometrically.
- (iii). Determination of the strength of strong and weak acids in a given mixture using a potentiometer/pH meter.
- (iv). Determination of temperature dependence of EMF of a cell.
- (v). Determination of the formation constant of silver-ammonia complex and stoichiometry of the complex potentiometrically.
- (vi). Acid-base titration in a non-aqueous media using a pH meter.

- (vii). Determination of activity and activity-coefficient of electrolyte.
- (viii). Determination of the dissociation constant of acetic acid in DMSO, DMF, acetone and dioxane by titrating it with KOH.
- (ix). Determination of the dissociation constant of monobasic/dibasic acid by Albert-Serjeant method.
- (x). Determination of thermodynamic constant ΔG , ΔS and ΔH for the reaction by EMF method. $\text{Zn} + \text{H}_2\text{SO}_4 \rightarrow \text{ZnSO}_4 + 2\text{H}^+$

C. Polarimetry:

- (i). Determination of rate constant for hydrolysis/inversion of sugar using a polarimeter.
- (ii). Enzyme kinetics-inversion of sucrose

Recommended Books:

1. Gurdeep, R. (2016). *Advanced Practical Inorganic Chemistry*, revised Ed., Krishna Prakashan publication.
2. Svehla, G. (2010). *Vogel's Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall.
3. Gurtu, J. N. and Gurtu, A. (2011). *Physical Chemistry Vol – I*, Pragati Prakashan publication.
4. Leonard, J., Lygo, B., & Procter, G. (2013). *Advanced Practical Organic Chemistry* (3rd ed.). CRC Press, Taylor & Francis Group.
5. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. (1989). *Practical Organic Chemistry* (5th ed.). New York, John Wiley & Sons, Inc.
6. Gurtu, G.N., Gurtu, A. (2014). *Advanced Physical Chemistry*, India: Pragati Prakashan.
7. Sindhu, P.S. (2005). *Practicals in Physical Chemistry*, India: Macmillan Publishers.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>

3. Free Online Education SWAYAM

<https://swayam.gov.in>

Third Semester

CHEM 514 Bioinorganic and Bioorganic Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- discuss structures and properties of carbohydrates, amino acids and proteins.
- understand metalloenzymes, mechanism of action of enzymes and their role in biological process.
- explain the structures of haemoglobin, myoglobin and mechanism of dioxygen transport in living system.
- elaborate electron transport chain and its role in energy generation, nitrogen fixation and photolysis of water.
- explain the structures of different biomolecules through model complexes of iron, cobalt and copper.

Section-A

Carbohydrates:

Isomerism, mutarotation, oxidation, reduction, glycoside formation, osazone formation, synthesis and degradation of monosaccharides, configuration of D-glucose, general discussion of disaccharides and polysaccharides, identification tests for carbohydrates

Amino Acids and Proteins:

Classification, identification, general methods of preparation and reactions of amino acids; primary, secondary, tertiary and quaternary structure of protein; analysis of polypeptides and proteins

Mechanism of Enzyme Action:

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion, examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease and lysozyme

Section-B

Metal Ions in Biological Systems:

Na^+ / K^+ pump, toxic metal ions and their detoxification, chelation therapy/chelating agents in medicine

Transport and Storage of Dioxygen:

Heme proteins and oxygen uptake, structure and function of hemoglobin, myoglobin, hemocyanin and hemerythrin, models of synthetic complexes of iron, cobalt and copper.

Metalloenzymes:

Zinc enzymes: carboxypeptidase and carbonic anhydrase; copper enzyme: superoxide dismutase; xanthine oxidase, vitamin B12, Iron enzymes: catalase, peroxidase and cytochrome P-450.

Section-C

Electron Transfer in Biological Systems:

Structure and function of metalloproteins in electron transport processes, cytochromes and iron-sulphur proteins and synthetic models

Metalloproteins in Energy Transmission:

Metal complexes in transmission of energy, structure and reactivity of chlorophylls, photosystem-I and photosystem-II in cleavage of water, model systems.

Biological Nitrogen Fixation:

Fixation of nitrogen biologically and non-biologically, spectroscopic and other evidences, transition metal sulphide models for nitrogenase sites, Fe-Mo-S cluster models for Fe-Mo-Co.

Recommended Books

1. Lippard, S.J. & Berg, L.M. (1994). *Principles of Bioinorganic Chemistry*. V.A.: University Science Books.
2. Bertini, I., Gray, H.B., Lippard S.J. & Valentine, J.S. (1994). *Bioinorganic Chemistry*. V.A.:University Science Books

3. Dugas, H., & Penny, C. (1981). *Bioorganic Chemistry: A Chemical Approach to Enzyme Action*. New York: Springer-Verlag.
4. Suckling, C.J. (1990). *Enzyme Chemistry: Impact and Application*. 2th Ed., London: Chapman & Hall.
5. Page, M.I. & Williams, A. (1987). *Enzyme Mechanisms*. London: Royal Society of Chemistry.
6. Price, N. & Stevens, L. (1999). *Fundamentals of Enzymology*. 3th Ed., Oxford: Oxford University Press.
8. Trevan, M.D. (1980). *Immobilized Enzyme: Introduction and Application in Biotechnology*. New York: John Wiley & Sons, Inc.
7. Walsh, C. (1981). *Enzymatic Reaction Mechanisms*. New York: WH Freeman & Co.
8. Fersht, A. (1985). *Enzyme Structure and Mechanism*. New York: WH Freeman & Co.
9. Lehninger, A.L. (1992). *Principles of Biochemistry*. India: CBS Publishers.
10. Voet, D., Voet, J.G. & Pratt, C.W. (1999). *Fundamentals of Biochemistry*. New York: John Wiley & Sons.
11. Mahler, H.R., & Cordes, E.H. (1971). *Biological Chemistry*, 3th Ed., New York: Harper and Row Publication.
12. Bruice, T.C., & Bentkovic, S. (1966). *Bioorganic Mechanisms, Vol. I & II*, New York: Benjamin WA.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 516D Literature Dissertation

Max. Marks : 100	L	T	P	C
(CA: 40 + ESA: 60)	0	0	8	4

Learning Outcomes:

On completion of course, the students will be able to:

- survey literature in systematic manner.
- present information and write reports in a clear, effective and scientific manner.
- develop their skills for future research.

Topics will be allotted to students by concerned teacher/teachers.

CHEM 509 Organic Chemistry (Chemistry of Natural Products)

Max. Marks : 100	L	T	P	C
(CA: 40 + ESA: 60)	4	0	0	4

Learning Outcomes:

On completion of course, the students will be able to:

- explain the synthesis and biogenesis of terpenoids, carotenoids, alkaloids, steroids, porphyrins, prostaglandins and flavanoids.
- elucidate the structures of terpenoids, alkaloids, steroids and flavonoids.
- identify natural products and their probable biosynthetic pathways.
- understand the key metabolic pathways.

Section-A

Terpenoids and Carotenoids:

Classification, nomenclature, occurrence, isolation, identification (qualitative idea only), general methods of structure determination, isoprene rule, special isoprene rule, structure determination, stereochemistry and synthesis of the following representative molecules: - citral, α -pinene, α -terpeneol, abietic acid and β -carotene.

Porphyrins:

Structure and synthesis of hemoglobin and chlorophyll (for structure elucidation, emphasis is to be placed on the use of spectral parameters whenever possible).

Section-B**Alkaloids:**

Definition, nomenclature and physiological action, occurrence, isolation, identification (qualitative idea only), general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants; structure, stereochemistry and synthesis of the following: coniine, nicotine, atropine, quinine and morphine.

Prostaglandins:

Occurrence, nomenclature, classification, biogenesis and physiological effects and synthesis of PGE₂ and PGF_{2a}.

Section-C**Steroids and Hormones:**

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry, isolation, identification (qualitative idea only), structure determination and synthesis of cholesterol, androsterone, testosterone, oestrone, progesterone.

Plant Pigments:

Occurrence, nomenclature and general methods of structure determination, isolation and synthesis of apigenin, luteolin, cyanidin, daidzein, gennistein and hirsutidin.

Key Metabolism Pathway:

Acetate pathway, mevalonate pathway and shikimic acid pathway.

Recommended Books

1. Mann, J., Davidson, R.S., Hobbs, J.B., Banthrope, D.V., & Harborne, J.B. (1994). *Chemistry and Biological Significance*. New York : Wiley publication.
2. Finar, I. L. (1964). *Stereochemistry and the chemistry of natural product* (3rd ed.). London: Longmanns.

- Hostettmann, E.K., Gupta, M.P., & Marston, A. (1999). *Chemistry, Biological & Pharmacological Properties of Medicinal Plants from the Americas*. The Netherlands: Harwood Academic Publishers.
- Bohm, B.A. (1998). *Introduction to Flavonoids*. The Netherlands: Harwood Academic Publishers.

Suggested e-Sources

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- Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
- Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 521 Physical Spectroscopy

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- understand the principles of advanced spectroscopic techniques.
- understand the Raman effect and rotational vibrational Raman spectra used for the structure determination.
- calculate the bond length of compounds and reduced mass by microwave spectroscopy
- calculate binding energy of electrons .
- explain the X-ray diffraction and measurements, and band theory of conductance.

Section-A

Rotational (Microwave) Spectroscopy:

Principal moment of inertia, classification of rotors: rigid rotor and non rigid rotor, selection rule (rigid rotor), effect of isotopic substitution frequencies, linear polyatomic molecules, non-linear polyatomic molecules,

asymmetric Top molecules, relative intensities of spectral lines, stark effect, nuclear and electron spin interaction, instrumentation and application.

Raman Spectroscopy:

Raman Effect, theory of Raman Effect (quantum mechanical and classical), rotational Raman spectra, vibrational Raman spectra, rule of mutual exclusion and structure determination, instrumentation, presentation of spectra, determination of depolarization ratio (ρ_n) and application.

Section-B

Photo Electron Spectroscopy (PES):

Principles of photoelectron spectroscopy, PES and Koopman's theorem, types of PES, photo ionization constant, chemical shift in Electron Spectroscopy for Chemical Analysis (ESCA), instrumentation, techniques of PES, atomic and molecular electron spectra, application of ESCA.

Electron Diffraction:

Principle, scattering intensity and scattering angle, Wierl equation, measurement techniques, Elucidation of simple gas phase molecules, low energy electron diffraction (LEED) and structure surfaces, application of electron diffraction.

Neutron Diffraction:

Theory of neutron diffraction, scattering of neutron by solid and liquids, magnetic scattering, measurement techniques, elucidation of structure of magnetically ordered unit cell, application of neutron diffraction.

Section-C

Laser Spectroscopy:

Types of laser: solid-state laser, continuous-wave (cw) laser, neodymium laser, helium neon laser, carbon dioxide laser, argon-ion krypton ion laser, Chemical laser, frequency doubling application of laser: Raman spectroscopy, resonance-ionisation spectroscopy.

The Solid State:

Classification, Symmetry, point groups, Bravais Lattice, lattice energy (Born-lande equation), law of rational indices, Miller indices, X-ray diffraction and measurement (The Debye-Scherrer Method), band theory of

conductors, semiconductors and insulators, extrinsic semiconductors, superconductivity, effect of temperature on superconductivity.

Recommended Books

1. Atkin's, P., Julio, P. D., (2014). *Physical Chemistry* (10th ed.), U. K., Oxford University Press.
2. Banwell, C.N., & Mc Cash, Elaine M., (1983) *Fundamental of molecular spectroscopy* (3rd ed.), UK. Mc Graw-Hill Companies.
3. Kaur, H., (2017) *Spectroscopy*, India, Pragati Prakashan.
4. Puri, B.R., Sharma, L.R., Pathania. M.S. (2016). *Principle of Physical Chemistry* (47th ed.), India, Vishal Publishing Company.
5. Barrow, G.M., (1962) *Introduction to molecular spectroscopy*.USA, Mc Graw-Hill Companies.
6. Hollas, J.M., (2004). *Modern spectroscopy* (4th ed.), USA, John Wiley & Sons Ltd.
7. Brown, J. M., (2003). *Rotational spectroscopy of diatomic molecules*, UK, Cambridge University Press.
8. West, A. R, (2014). *Solid State Chemistry and its Applications* (2nd ed.), John Wiley & Sons Ltd.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 505L Chemistry Lab -III

Max. Marks : 100	L	T	P	C
(CA: 40 + ESA: 60)	0	0	12	6

Learning Outcomes:

On completion of course, the students will be able to:

- develop their skills for qualitative and quantitative research in different fields.
- perform various analytical operations to qualify and quantify different analytes.
- outline synthetic strategies for important chemicals.
- check the purity of synthesized compounds through TLC, conductance and magnetic susceptibility measurements, and UV, FT-IR spectral data.

Inorganic Chemistry

I. Estimation and Separation:

1. Estimation of Nitrogen by Kjeldahl's Method.
2. Estimation of Sulphur/Halogen by Fusion Method.
3. Determination of boric acid in borax.
4. Determination of metals: copper in copper oxychloride and zinc in zineb fungicides.
5. Separation of Cu, Co and Zn on paper strips.
6. Separation of Cu and Ni on cellulose column.
7. Separation and determination of Zn and Cd using Ion Exchanger.
8. Separation and determination of Co and Ni using Ion Exchanger.
9. Separation and determination of chloride and bromide using Ion Exchanger.
10. Separation and spectrophotometric determination of Cu, Fe, and Ni using Ion Exchanger.
11. Separation and determination of Cl^- and I^- (aqueous-acetone medium).

II. Solvent Extraction:

1. Determination of Fe(III) by chloride extraction in ether.
2. Determination of Fe(III) as the 8-hydroxy quinolate (oxinate) by extraction in chloroform.

Organic Chemistry

Qualitative Analysis

Separation, purification and identification of the components of a mixture of three organic compounds (three solids, two liquids and one solid, two solids and one liquid) using the chemical analysis.

Three-steps Organic Synthesis

The exercises should illustrate the use of organic reagents and may involve purification of the products by chromatographic techniques:

1. Benzophenone → Benzophenoneoxim → Benzanilide → Benzoic acid + Aniline
2. Aniline → Acetanilide → *p*-nitroacetanilide → *p*-nitroaniline
3. Glucose → D-glucosepentacetate → Glucose → 1-methylglucose

Physical Chemistry

Electrochemistry:

1. Titrate a mixture of copper sulphate, acetic acid and sulphuric acid with sodium hydroxide.
2. Titrate phosphoric acid potentiometrically against sodium hydroxide.
3. Determine the dissociation constant (pKa) of a weak acid using pH meter.
4. Determine the Hammett constant of a given substituted benzoic acid by pH measurement.
5. Determine the acidic and basic dissociation constant of an amino acid and the isoelectric point of an acid.
6. To determine the hydrolysis constant of aniline hydrochloride by pH measurement.

Magneto Chemistry:

1. To determine the magnetic susceptibility of a given compound and calculate the number of unpaired electrons present in it.
2. To verify the Weidemann's law using nickel chloride solution.

Colorimetric:

1. To determine equilibrium quotient for the formation of monothiocynato iron(III) complex by colorimetric measurement.
2. Investigate the reaction kinetics between potassium persulphate and potassium iodide by colorimetric measurement.
3. Determine the concentration of Cu^{2+} ions in given solution titrating with EDTA solution by colorimetric measurement.

Phase Equilibrium:

1. To draw the mutual solubility curve of two immiscible liquid and find out the critical solution temperature of phenol-water system.
2. To obtain the phase diagram of water-ethanol-benzene system at room temperature.

Potentiometry:

1. To find out the strength of cobalt sulphate solution by titrating it against a standard solution of potassium ferricyanide.
2. To determine the solubility and solubility product of sparingly soluble salt.

Polarography:

1. To plot a polarogram for a mixed solution of Cd^{2+} , Zn^{2+} and Mn^{2+} ions in 0.1 M KCl.
2. To determine the half wave potential of Cd^{2+} , Zn^{2+} ion in 0.1 M KCl.

Recommended Books

1. Gurdeep, R (2016), *Advanced Practical Inorganic Chemistry*, revised Ed., Krishna Prakashan publication.
2. Svehla, G. (2010), Vogel's *Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall.
3. Gurtu, J. N. and Gurtu, A(2011), *Physical Chemistry Vol – I*, Pragati Prakashan publication.
4. Leonard, J., Lygo, B. & Procter, G. (2013), *Advanced Practical Organic Chemistry* (3rd ed.). CRC Press, Taylor & Francis Group.

5. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. (1989). *Practical Organic Chemistry* (5th ed.). New York, John Wiley & Sons, Inc.
6. Gurtu, G.N., Gurtu, A. (2014). *Advanced Physical Chemistry*, India: Pragati Prakashan .
7. Sindhu, P.S. (2005). *Practicals in Physical Chemistry*, India: Macmillan Publishers.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

Fourth Semester

CHEM 501 Advanced Inorganic Chemistry

Max. Marks : 100	L	T	P	C
(CA: 40 + ESA: 60)	4	0	0	4

Learning Outcomes:

On completion of course, the students will be able to:

- explain the principles and concepts of Green Chemistry.
- minimize the use of organic solvents by using solvent-free reactions and supercritical fluids.
- predict the structure, bonding of metal carbonyls, metal nitrosyl, dinitrogen and dioxygen complexes, vibrational spectra of metal carbonyls for bonding and structural elucidation.
- apply the principles of biomimetic chemistry in design and synthesis of receptors for recognition of various hosts: cationic, anionic and neutral; supramolecular reactivity, catalysis and supramolecular devices.

Section-A

Principles and concepts of Green Chemistry:

Introduction, definition, principles, atom economy, atom economic and atom uneconomic reaction, reducing toxicity, waste minimization techniques, on-site waste treatment, design for degradation, polymer recycling.

Catalysis and Green Chemistry:

Introduction to catalysis, heterogeneous catalysis-basics, zeolites, sulfonated resins, clays, oxidation, catalytic converters; homogeneous catalysis-transition metal catalysis, asymmetric catalysis; phase transfer catalysis, bio catalysis, photo catalysis.

Green Solvents:

Organic solvents, solvent-free systems, controlling of solvent-free reactions, supercritical fluids (H_2O and CO_2)-introduction, extraction, advantages and applications; ionic liquids-synthesis.

Section-B

Metal π -Complexes-I:

Metal carbonyls:-preparation, important reactions, structure, bonding, vibrational spectra of metal carbonyls for bonding and structural elucidation.

Metal π -Complexes-II:

Structure and important reaction of transition metal nitrosyl, dinitrogen and dioxygen complexes, tertiary phosphine as a ligand.

Metal Clusters:

Higher boranes, carboranes, metalloboranes and metallocarboranes, compounds with metal-metal multiple bonds, metal carbonyl and halide clusters.

Section-C

Supramolecular Chemistry:

Molecular recognition, supra molecular interactions, molecular receptors for different types of molecules including cationic and anionic guests, crown ether and cyclodextrins receptors: synthesis and applications, design

and synthesis of co-receptor molecules and multiple recognition, supramolecular devices: - photonic, electronic and ionic devices

Recommended Books

1. Lancaster, M., (2002) *Green chemistry: an introductory text*:Royal society of chemistry.
2. Paul, T. Anastas., Tracy, C. Williamson. (1998). *Green Chemistry: Frontiers in Benign Chemical Synthesis and Processes*:oxford university press.
3. Paul, T. Anastas., & Lauren G. H.(2000).*Green Chemical Syntheses and Processes*: vol 767, ACS Symposium Series.
4. Cotton, F.A., & Wilkinson, G. (1999). *Advanced inorganic chemistry*,6th ed:John Wiley.
5. Huhey, J.E.(1978).*Inorganic Chemistry*: Harpes & Row.
6. Lippard.S.J., & Berg. J. M.*Principle of Bioinorganic Chemistry*: University Science Books, Mill Valley.
7. Bertini, I.H.B., Gray.S.J.V, *Bioinorganic Chemistry*: University Science Books, Mill Valley.
8. Eichhorn, G.L.(2007). *Inorganic Biochemistry*, Vols I, II. Ed: Elsevier
9. Lehn, J.M (2006).*Supramolecular Chemistry*: Wiley and VCH.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 502 Advanced Physical Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- understand the oscillatory reactions, rate equations of different types of reactions, and thermodynamic excess function of non ideal solutions.
- explain the Maxwell-Boltzman, Fermi-Dirac and Bose-Einstein statistics.
- explain the concept of entropy productions and Onsager's reciprocity relation.
- understand the basics of electrochemistry and polarography.
- explain the structure of electrified interface, and double layer parallel-plate condenser models.

Section-A

Oscillatory Reactions:

Autocatalysis and oscillatory reactions, Kinetics and mechanism of Belousov-Zhabotinski (B-Z) reactions

Thermodynamics:

Thermodynamics of non-ideal solutions, chemical potential in non-ideal solution, excess functions of non-ideal solutions, experimental determination of excess function, calculation of partial molar quantities from experimental data.

Chemical Kinetics:

Mechanism of Composite Reactions - types of composite mechanisms, rate equations for composite mechanisms, simultaneous and consecutive reactions, steady state treatment, rate-determining steps, microscopic reversibility dynamic chain ($\text{H}_2\text{-Br}_2$ reaction, decomposition of ethane and acetaldehyde).

Section-B

Statistical Thermodynamics:

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical, grand canonical and micro-canonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translation, rotational, vibrational and electronic partition functions, Calculation of thermodynamic properties in terms of partition. Application of partition functions. Heat capacity behaviour of solids-chemical equilibria and equilibrium constant in terms of partition functions, Fermi-Dirac Statistics, distribution law, Bose-Einstein statistics distribution Law.

Non-Equilibrium Thermodynamics:

Thermodynamic criteria for non-equilibrium states, entropy production, entropy production in heat flow and matter flow, entropy production in chemical reaction. The phenomenological law, microscopic reversibility and Onsager's reciprocity relations transformations properties of the generalized fluxes and forces, non-equilibrium stationary states (Prigogine's principle of minimum entropy production), electro kinetic phenomena, diffusion.

Section-C

Electrochemistry:

Electrochemistry of solutions, activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions, determination of activity and activity coefficient by EMF methods (with and without). Debye-Huckel-Onsager treatment and its extension, ion solvent interactions: thermodynamics of electrified interface equations, Lippmann equations (surface excess), determination of surface excess, structure of electrified interfaces double layer: parallel-plate condenser model (Helmholtz-Perrin theory), Guoy-Chapman model, Stern model, exchange current density, derivation of Butler-Volmer equation, equation of tunneling, Wentzel, Kramer and Brillouin(WKB) approximation, polarography theory, Ilkovic equation; half wave potential and its significance.

Recommended Books

1. Bard, A. J., Faulkner, L. R. (2002) *Electrochemical Methods: Fundamentals and Applications*, (2nd ed.), New York, John Wiley & Sons.
2. Bockris, J. O' M., Reddy, A. K. N. (1998) *Modern Electrochemistry 1: Ionics* (2nd ed.), USA, Springer.
3. Bockris, J. O' M., Reddy, A. K. N. & Gamboa-Aldeco, M. E. (2001). *Modern Electrochemistry 2-A: Fundamentals of Electrode Processes* (2nd ed.), USA Springer.
4. Bockris, J. O' M. & Reddy, A. K. N. (2001). *Modern Electrochemistry 2-B: Electrode Processes in Chemistry, Engineering, Biology and Environmental Science* (2nd ed.), USA, Springer.
5. Brett, C. M. A. & Brett, A. M. O. (1993). *Electrochemistry-Principle, methods and application*, UK, Oxford University Press.
6. Koryta, J., Dvorak, J. & Kavan, L. (1993). *Principles of Electrochemistry*, New York, John Wiley & Sons.
7. Pilling, M. J. & Seakins, P. W. (1997). *Reaction Kinetics*, UK, Oxford Press.
8. Laidler, K.J., (1965) *Chemical Kinetics* (2nd ed.), New York, McGraw Hill Book Company.
9. Atkin's, P., Julio, P. D., (2014). *Physical Chemistry* (10th ed.), U. K., Oxford University Press.
10. Puri, B.R., Sharma, L.R., Pathania. M.S. (2016). *Principle of Physical Chemistry* (47th ed.), India, Vishal Publishing Company.
11. Groot, SR. de., Mazur, P., (1962) *Non- Equilibrium Thermodynamics*, Amsterdam, North-Holland Publishing Company.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
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3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 510 Organic Synthesis

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- understand the fundamentals of organic synthesis such as disconnection approach of 1,3-difunctional and 1,5-difunctional compounds
- apply the concepts of microwave assisted synthesis in various organic reactions.
- apply the mechanistic aspects of various name reactions in synthetic organic chemistry.

Section-A

Fundamentals of organic synthesis:

Disconnection approach, one group and two group disconnections, reversal of polarity, one group C-C disconnection, two group C-C disconnections, 1,3-difunctional and 1,5-difunctional compounds, tandem reactions, domino reactions and multi-component reactions.

Microwave Synthesis:

Fundamental theory, mechanism of microwave heating, application of microwave heating, polarization, types of reactions, choice of solvents, reaction vessels, functional group transformation, condensation, oxidation, reduction. Name reactions:-Friedel-Crafts reaction, Fischer-indole reaction, Reformatsky reaction, Perkin reaction, Cannizzaro reaction, Mannich reaction, Michael addition, Claisen-schmidt condensation, Knoevenagel condensation and Gabriel condensation.

Section-B

Oxidation:

Introduction, different oxidative processes, hydrocarbons: -alkenes, saturated C-H groups (activated and inactivated); alcohols and diols; aldehydes and ketones; oxidations with ruthenium tetroxide, iodobenzene diacetate and thallium (III) nitrate.

Reduction:

Introduction, different reductive processes, hydrocarbons: - alkenes, alkynes and aromatic rings; carbonyl compounds: aldehydes, ketones; acids and their derivatives; epoxides; hydrogenolysis.

Section-C**Rearrangements:**

General mechanistic considerations, nature of migration, migratory aptitude, memory effects, a detailed study of the following rearrangements:- pinacol-pinacolone, Wagner-Meerwein, Tiffeneu-Demjanov, Beckmann, Hofman, Curtius, Lossen, Schmidt, Baeyer-Villiger, 74benzyl-benzilic acid, Favorskii, Neber, benzidine and Fries rearrangement.

Name reactions:

Discuss in detail to following name reactions with reference to their application in the synthesis of some medicinal agents, where possible: - Friedel-Crafts reaction, Darzen's condensation, Dieckmann's condensation, Willegordt reaction and Arndt-Eistert synthesis.

Organoboron Compounds: Structure, synthesis and applications of organoboron compounds.

Recommended Books

1. Smith, M. B., March, J. (2007). *Advanced Organic Chemistry Reaction Mechanism and Structure*. A John Wiley & Sons (6th ed.).
2. Carey, F. A. Sundberg, R. J. (2007). *Part A : Structure and Mechanism*. Springer (5th ed.).
3. House, H. O., Benjamin, W. A.(1965). *Modern Organic Reactions*. W.A Benjamin New York.
4. Clayden, J., Greeves, N., Warren, S., Wothers, P.(2001). *Organic chemistry*. Oxford University Press (2nd ed.).
5. Sykes, P. (1986). *A guide book to mechanism in organic chemistry* (6th ed.).
6. Ingold, C. K.(1970). *Structure and mechanism in organic chemistry*. Cornell University Press.
7. Morrison, R.T.,Boyd, R.N. (2002). *Organic chemistry* (6th Ed.).

8. Nasipuri, D.(1994). *Stereochemistry of organic compounds*. New Age International (2nd ed.).
9. Singh, M.S, (2005). *Advanced organic chemistry-reactions and mechanisms*. Pearson Education (Singapore) Pvt. Ltd.
10. Wade, L.G., Singh, M.S. (2008). *Organic chemistry*. Pearson Education, (Dorling Kindersley Pvt. Ltd.
11. Singh, M.S. (2014). *Reactive intermediates in organic chemistry-structure, mechanism and reactions*. Wiley, VCH, & Weinheim.

Suggested e-Sources:

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2. Online Chemistry Courses
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<https://swayam.gov.in>

CHEM 511 Organotransition - Metal Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- use the basic principles of descriptive chemistry and molecular orbital theory to describe the chemical bonding and structure of organometallic compounds.
- explain and predict the chemical behavior and reactivity of organometallic compounds.
- describe and explain the catalytic processes using an organometallic compound as a catalyst.
- explain the uses of organometallic compounds as catalysts in organic synthesis

Section-A

Alkyls and Aryls of Transition Metals:

Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

Compounds of Transition Metal-Carbon Multiple Bonds:

Low valent carbenes, alkylidenes, carbynes and alkylidyne:-synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligand, role in organic syntheses.

Section-B

Transition Metal π -Complexes:

Transition metal π -complexes with unsaturated organic molecules: - alkenes, alkynes, allyl, diene, dienyl, arene and trienyl complexes; preparations, properties, nature of bonding and structural features, important reactions relating to nucleophilic and electrophilic attack on ligands and role in organic syntheses, transition metal compounds with bonds to hydrogen.

Section-C

Homogeneous Catalysis:

Fundamental reaction steps of transition metal catalyzed reactions, stoichiometric reactions for catalysis, homogeneous catalytic hydrogenation, Zeigler-Natta polymerization of olefins, catalytic reactions involving carbon monoxide such as hydrocarbonylation of olefins (oxo reaction), oxopalladation reactions, activation of C-H bond.

Heterogeneous Catalysis: Fischer Tropsch process: methanation reaction, synthesis of methanol, gasoline production, water gas shift reaction, role of ZnO/Cr_2O_3 in the reaction, acetic acid synthesis, role of CO catalyst.

Fluxional Organometallic Compounds:

Fluxional and dynamic equilibria in compounds such as η^1 -olefin, η^3 -allyl and dienyl complexes.

Recommended Books

1. Collam, J.P., Hegedus, L.S., Norton, J.R., & Finke, R.G. (1988). *Principle and Application of Organotransition Metal Chemistry*. Oxford: Oxford university press.

- Crabtree, R.H. ((2008).*The Organometallic Chemistry of the Transition Metals* (6th ed.). New Jersey: John Wiley publications.
- Mehrotra ,R.C. & Singh, A.(2000) *Oraganometallic Chemistry* . New Delhi: New Age International.

Suggested e-Sources

- National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
- Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
- Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 506L Chemistry Lab-IV

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

0 0 12 6

Learning Outcomes:

On completion of course, the students will be able to:

- develop their skills for qualitative and quantitative research in different fields.
- perform various analytical operations to qualify and quantify different organic and inorganic samples.
- elucidate the structures of organic compounds by UV, FT-IR, Mass and NMR spectral data.
- present information and write reports in a clear, effective and scientific manner.

Inorganic Chemistry:

- Quantitative analysis of tri-component mixture of metal ions gravimetrically, volumetrically and spectrophotometrically.
 - Mixed solution of Cu^{2+} - Ni^{2+} - Zn^{2+}
 - Mixed solution of Cu^{2+} - Ni^{2+} - Fe^{3+}
- Spectrophotometric determination:

- (i). Manganese / Chromium / Vanadium in steel sample.
 - (ii). Iron-phenanthroline complex: Job's method of continuous variation.
 - (iii). Zirconium-Alizarin red complex: Slope ratio method.
 - (iv). Phosphate, Nitrite, Fluoride and Sulphate
3. Analysis of dolomite.
 4. Analysis of brass.
 5. Colorimetric determination of chromium (VI) (in ppm) using 1,5 diphenyl carbazide as a reagent for colour development.

Organic Chemistry:

1 Column Chromatography

Separation of typical binary solid mixtures of organic compounds by column chromatography.

2. Paper Chromatography

Separation and identification of the sugars present in the given mixture of glucose, fructose and sucrose by paper chromatography and determination of R_f values.

3. Spectroscopy

Identification of organic compounds by the analysis of their spectral data (UV, IR, PMR, CMR & MS)

4. Spectrophotometric (UV/VIS) Estimations:

- (i). Amino acids
- (ii). Proteins
- (iii). Carbohydrates
- (iv). Cholesterol
- (v). Ascorbic Acid

Physical Chemistry**Chemical Kinetics:**

1. To find out the velocity constant of reaction between potassium persulphate and potassium iodide and also calculate the activation energy, and the influence of ionic strength on rate constant.

2. To study the reaction between acetone and iodine in the presence of acid.

Solution:

1. To study the variation of solubility of potassium hydrogen tartrate with ionic strength using a salt having common ion and determine the mean ionic activity coefficient.
2. To study the effect of ionic strength on the solubility of calcium sulphate and determine its thermodynamic solubility product.

Adsorption:

1. Adsorption of acetic acid on charcoal to verify Freundlich and Langmuir's isotherm.
2. To study the adsorption of oxalic acid on charcoal and to prove the validity of Freundlich and Langmuir's isotherm.
3. To study the adsorption of iodine from alcoholic solution on charcoal.

Partition Coefficient

1. To find out the equilibrium constant of tri-iodide formation.
2. To find out the dimerization constant of benzoic acid in benzene.
3. To find the formula of complex copperammonium ion or study the complex formation between copper sulphate and ammonia solution.
4. To study the complex formation and find the formula of silver amine complex by partition method.

Recommended Books

1. Gurdeep, R (2016), *Advanced Practical Inorganic Chemistry*, revised Ed., Krishna Prakashan publication.
2. Svehla, G. (2010), Vogel's *Qualitative Inorganic Analysis*, 7th Edition, Prentice Hall.
3. Gurtu, J. N. and Gurtu, A(2011), *Physical Chemistry Vol – I*, Pragati Prakashan publication.
4. Leonard, J., Lygo, B. & Procter, G. (2013), *Advanced Practical Organic Chemistry* (3rd ed.). CRC Press, Taylor & Francis Group.

5. Furniss, B.S., Hannaford, A.J., Smith, P.W.G. & Tatchell, A.R. (1989). *Practical Organic Chemistry* (5th ed.). New York, John Wiley & Sons, Inc.
6. Gurtu, G.N., Gurtu, A. (2014). *Advanced Physical Chemistry*, India: Pragati Prakashan.
7. Sindhu, P.S. (2005). *Practicals in Physical Chemistry*, India: Macmillan Publishers.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

Discipline Elective Papers:

CHEM 519 Nanomaterials

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- understand nanomaterials and their properties.
- fabricate nanomaterials and characterize them.
- explain the stability of nanomaterials.

Section-A

Introduction to nano, emergence and challenges in nanotechnology, properties of nanomaterials; classification of nanomaterials: one dimensional, two dimensional and three dimensional; quantum dots, core-shell nanostructures, nanocomposite, nanowires, nanorods, new form of carbon (carbon nanotubes, grapheme and fullerenes).

Section-B

Fabrication of Nanomaterials:

Bottom-up approaches: Chemical reduction method, sol-gel process and chemical vapor deposition, and top-down approaches: ball milling, and lithography.

Stability of Nanomaterials:

Surface energy, surface area and surface area to volume ratio, stabilisation of nanoparticles: electrostatic stabilization with special reference to DLVO theory, steric stabilization and electrosteric stabilization.

Section-C

Characterization Techniques of Nanomaterials:

Principle and instrumentation of X-ray diffraction, small angle X-ray scattering, field emission scanning electron microscopy, transmission electron microscopy, surface area analyzer.

Applications of Nanomaterials: Representative Examples

In the field of health and medicine, environment, energy, catalysis and agriculture.

Recommended Books:

1. Cao, G. (2004). *Nanostructures and nanomaterials: synthesis, properties and application*. Empirical College Press.
2. Geoffrey, A. Ozin, (2005). *Nanochemistry: A chemical approaches to nanomaterials*. Royal Society of Chemistry.
3. Gabor, L. H., Harry, F. T., Dutta, J., Moore, J.J. (2008). *Introduction to nanosciences & nanotechnology*. CRC Press Taylor & Francic group.
4. Guozhong, C. (2011). *Nano structure & nanomaterials synthesis, properties & application*. Imperial College Press.
5. Pradeep, T. (2007). *Nano: The essentials*. McGraw Hill Pvt. Ltd.
6. Shah, M.A., Shah, K.A. (2013). *Nanotechnology: The science of small*. Wiley Publication.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 512 Photo-organic and Heterocyclic Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- demonstrate advanced knowledge and understanding in aspect of photochemical reactions.
- introduce about basic chemistry of the heterocyclic.

- The students will get familiar with particular properties and reactions for the most important heterocyclic as well as different systems of nomenclature.
- The students will develop fundamental theoretical understanding of heterocyclic chemistry.
- fully comprehend the chemistry of many heterocyclic products, in use such as drugs and food.

Section-A

Photochemistry-I:

Photochemical reactions: interaction of electromagnetic radiation with matter, types of excitations, fate of excited molecule, quantum yield, transfer of excitation energy, photochemistry of alkenes:- intramolecular reactions of the olefinic bond, geometrical isomerism, cyclisation reactions, rearrangements of 1,4- and 1,5-dienes; photochemistry of carbonyl compounds:- saturated, cyclic, acyclic, α,β -unsaturated and β,γ -unsaturated compounds, cyclohexadienones, intramolecular cycloaddition reactions:- dimerisations and oxetane formation.

Section-B

Photochemistry-II:

Photochemistry of aromatic compounds: isomerisation, additions and substitutions; miscellaneous photochemical reactions: - Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, singlet molecular oxygen reactions.

Heterocycle-I:

Small-ring heterocycles: three-membered and four membered heterocycles- synthesis and reactions of aziridines, oxiranes, azetidines and oxetanes; synthesis, reactions and application of imidazole, isooxazole, indole and benzofuran.

Section-C

Heterocycle-II:

Synthesis, reactions and applications of coumarins, thiocoumarins and chromones.

Synthesis, reactions and applications of pyridazine, pyrazine and pyrimidine;

Synthesis and reactions of 1,4- and 1,5-benzodiazepines.

Recommended Books

1. Rohtagi, K.K., Mukherji (1978). *Fundamentals of Photochemistry*, India: Wiley-Eastern, New Delhi.
2. Gilbert, A., Baggott, J. (1991). *Essentials of Molecular Photochemistry*. Oxford : Blackwell Scientific Publication.
3. Coxon, J., Halton, B. (1974). *Organic Photochemistry*. UK: Cambridge University Press.
4. Gupta, R.R., Kumar, M., Gupta, V. (1999). *Heterocyclic Chemistry, Vol. 1-3*, Berlin, Germany : Springer Verlag.
5. Joule, J.A., Mills, K., Smith, G.F. (1995). *Heterocyclic Chemistry*, London : Chapman & Hall.
6. Gilchrist, T.L. (1992). *Heterocyclic Chemistry*, New York : Longman Scientific Technical, Wiley.
7. Acheson, R.M. (1967). *An Introduction to the Heterocyclic Compounds*, New York : John Wiley & Sons.
8. Katritzky, A.R., Rees, C.W. (1984). *Comprehensive Heterocyclic Chemistry*, England : Pergamon Press.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 522 Polymer Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

On completion of course, the students will be able to:

- explain the various polymerization processes.
- understand the synthesis and properties of different polymers.
- appreciate the importance of recycling and disposal of rubber and polyurethane waste.
- differentiate the synthesis properties and uses of various inorganic polymers.

Section-A

Organic Polymers: Introduction, classification of polymers, types and mechanisms of polymerization: condensation polymerization, radical chain polymerization, ionic chain polymerization and copolymerization; molecular weight determination: principle, advantages and limitations; properties and applications of polymers.

Section-B

Synthesis and Properties of: Polyethylene, polyimides, polyacrylonitriles, polyvinyl alcohol, polymethylmethacrylate, polyvinyl acetate, phenol formaldehyde resin.

Conducting Polymer: Introduction and classification, polyacetylene, polyaniline, PEDOT, photo conducting polymers.

Recycling of Rubber Tyres and Polyurethane: Recycling and disposal of polyurethane and rubber.

Section-C

Inorganic Polymers: Classification, types of inorganic polymerization, comparison with organic polymers, co-ordination polymers, boron-oxygen and boron-nitrogen polymers, silicones, phosphorus-nitrogen, sulfur-nitrogen, sulfur-nitrogen-fluorine compounds.

Recommended Books

1. Goowarikar, V.R., Viswanathan, N.V., Sridhar, J. (1986). *Polymer science*, Halsted Press (John Wiley & Sons), New York.
2. Billmeyer, Fred W. (1984). *Text book of polymer science*. 3rd edition, Wiley-Blackwell.
3. Fried, Joel R. (2014). *Polymer science & technology*. 3rd edition, Prentice Hall.
4. Ghosh, P. (2010). *Polymer science and technology*. 3rd edition, McGraw-Hill India

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

ENVS 405 Environmental Chemistry

Max. Marks : 100

L T P C

(CA: 40 + ESA: 60)

4 0 0 4

Learning Outcomes:

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

- Describe the various chemical processes occurring in the air, water and soil.
- Explain the effect of hydrocarbons and synthetic compounds on biological organisms.
- Explain the degradation of hydrocarbon and synthetic compounds.
- Illustrate the working principle, merits and demerits of analytical techniques.

Course Content:

Section A

Concept and Scope of Environmental Chemistry: Definition and explanation for various terms, segments of environment. Principles and cyclic pathways in the environment: Sulphur, Oxygen, Nitrogen, Phosphorous cycle.

Chemistry of Water: Unusual physical properties, unusual solvent properties, changes in water properties by addition of solute.

Soil Chemistry: Formation, constituents and properties of soils, adsorption of contaminants in soil, soil fertility, surface exchange reaction, soil redox potential and adsorption-desorption.

Section B

Chemistry of various organic, inorganic, carcinogenic compounds and their effects. Hydrocarbons: Chemistry of hydrocarbon decay, environmental effects, effects on macro and micro organisms. Surfactants: Cationic, anionic and nonionic detergents, modified detergents.

Pesticides: Classification, degradation, analysis, pollution due to pesticides and DDT problems.

Synthetic Polymers: Microbial decomposition, polymer decay, ecological and consideration, Photosensitize additives.

Aflatoxin occurrence, chemical composition and properties metabolism.

Section C

Physico-Chemical methods for analysis of environmental samples: Definition and determination of conductivity, pH, COD, BOD.

Principle, merits and demerits of Centrifuge, and Ultra centrifuge.

Principle, merits and demerits of the techniques: colorimetry, atomic absorption spectroscopy, Atomic emission Spectroscopy, gas chromatography, HPLC, ion exchange chromatography.

Recommended Books:

1. Bhatia, S. C. (2006). *Environmental Chemistry*. New Delhi, India: CBS.
2. De, A. K., & De, A. K. (2007). *Environmental Chemistry*. New Delhi, India: New Age International.

3. Gary, W.V., & Stephen, J. D. (2010). *Environmental Chemistry. A global perspective*(3rded.). London, UK:Oxford University Press.
4. Rao, P. V. (2006). *Principles of Environmental Science and Engineering*. New Delhi, India:PHI.
5. Séamus, P. J. H. (2003). *Analytical Chemistry*. London, UK:Oxford University Press.
6. Manahan, S., &Manahan, S. E. (2009). *Environmental Chemistry (Ninth Edition)*. Florida, FL: CRC Press.
7. Wilson, K., &Walker, J. (2010). *Principals and Techiniques of Biochemistry and Molecular Biology*. New York, NY:Cambridge University Press.

Suggested e-learning materials:

1. Environmental Chemistry and Analysis <https://nptel.ac.in/courses/122106030/>
2. Environmental Chemistry
<https://swayam.gov.in/course/251-environmental-chemistry>
Syllabus pertains to ENVS 405 of Department of Environment Science

Reading Electives

CHEM 515R Forensic Science

Max. Marks : 100

(ESA: 100)

L	T	P	C
0	0	4	2

Learning Outcomes:

On completion of course, the students will be able to:

- appreciate the critical thinking and analysis abilities.
- develop laboratory skills to exacting standards to precision and care.
- apply diverse informations to solve real problems.

Forensic Science: Introduction and role of forensic science in crime investigation; types of cases/exhibits, preliminary screening, classification of physical evidence, presumptive test (colour and spot test), Examination procedures involving standard methods and instrumental techniques,

analysis of beverages: alcoholic, nonalcoholic and drugs as constituents.
Forensic document examination and finger print analysis.

Recommended Books

1. James, S. H., Nordby, J. J. (2005) *Forensic science: an introduction to scientific and investigative techniques*. CRC Press.
2. Siegel, J. A., Sukoo, R. J, Knupfer, G.C.(2000). *Encyclopedia of forensic science*. volume (I, II & III). Academic Press.
3. Brown, R., Davenport, J. (2012). *Forensic science: advanced investigations*. Cengage Learning.
4. Chadha, P.V.(2004). *Hand book of forensic medicine and toxicology*, New Delhi. NY: Jaypee Brothers.
5. Parikh, C.K. (1999). *Text book of medical jurisprudence forensic medicines and toxicology*. New Delhi. ND: CBS Pub.
6. Curry, A.S. (1986). *Analytical methods in human toxicology*. (Part II). CRC Press Ohio.

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 517R Metals in Medicines

Max. Marks : 100

L T P C

(ESA: 100)

0 0 4 2

Learning Outcomes:

On completion of course, the students will be able to:

- understand the role of metal complexes in the treatment of various disease.

- develop their insights for heavy metal toxicities and detoxification through chelation therapy.

Historical introduction to metals in medicine and key areas, Chelation therapy: Bertrand diagram, metal poisoning, the chelate effect, ligands used in chelation therapy, biologic considerations, Cis-platin: history, structure-reactivity relationships, aquation, biologic targets, DNA damage on adduct formation, DNA repair systems, biotransformation, side-effects, modes of resistance, 2nd generation Pt drugs: Carboplatin, oxaliplatin and nedaplatin modes of operation and side-effects, 3rd generation Pt drugs: sterically hindered Pt complexes, Pt(IV) complexes, complexes with biologically active carrier ligands, water soluble complexes, multinuclear Pt complexes, trans-Pt complexes.

Recommended Books

1. James, C. D. (2009). *Metals in medicine*. John Wiley & Sons, Ltd

Suggested e-Sources

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

CHEM 518R Nano Catalysis

Max. Marks : 100

(ESA: 100)

L	T	P	C
0	0	4	2

Learning Outcomes:

On completion of course, the students will be able to:

After completion of this course the student will be able to understand the basic mechanism of chemical reaction and the role of catalysis.

Review of techniques of interpretation of kinetic data, material and energy balance across reactors with reference to their design, Detail coverage of design of fixed, fluidized, trickle, moving bed reactors. Nanocatalysis: Role

of transition metals & metal oxides in homogeneous and heterogeneous catalysis and their mechanism of catalysis, manufacture of these catalysts in nano-form and their characterization. Silica, alumina, carbon as high temperature carriers for catalysts. Use of nanocatalysts in automobile pollution control, photocatalysis of toxics in effluents, gas sensors. Reactor design for manufacture of nanocatalysts and nanosupports: Design of flame aerosol reactors, diffusion and premixed flame reactors, co precipitation reactors, hot wall flow reactors; their mechanical features, modeling and simulations. Catalytic vapour –liquid- solid growth mechanism for understanding particle formation and growth during chemical vapour deposition, particle dynamics and CFD simulations of flame process based on fundamental equations for flow, heat and mass transfer, aerosol dynamics in flames.

Recommended Books

1. Levenspiel, O. (1999). Chemical reaction engineering. *Industrial & engineering chemistry research*, 38(11), 4140-4143..
2. Carberry, J. J. (2001). *Chemical and catalytic reaction engineering*. Courier Corporation.
3. Satterfield, C. N. (1970). *Mass transfer in heterogeneous catalysis*. The MIT Press.

Suggested –web resources

1. <https://ocw.mit.edu/search/ocwsearch.htm?q=%20nano%20catalysis>
2. <https://nptel.ac.in/courses/103108097/28>

CHEM 520R Pharmaceutical Chemistry

Max. Marks : 100

(ESA: 100)

L	T	P	C
0	0	4	2

Learning Outcomes:

- Develop understanding of drugs and their uses.
- Apply the concept of organic synthesis in drug synthesis.

Drugs and Pharmaceuticals: Drug discovery, design and development; basic retrosynthetic approach. Synthesis of representative drugs of following classes: analgesics agents, antipyretic agents, antiinflammatory agents (aspirin, paracetamol, Ibuprofen); antibiotics (chloramphenicol); antibacterial and antifungal agents (sulphonamides; sulphamethoxazol, sulphacetamide, trimethoprim); antiviral agents (acyclovir), central nervous system agents (phenobarbital), cardiovascular (glyceryl trinitrate), 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

Recommended Books:

1. Patrick, G.L. (2013). *Introduction to medicinal chemistry*, Oxford University Press, UK.
2. Singh, H., Kapoor, V.K. (2012). *Medicinal and pharmaceutical chemistry*, New Delhi. ND: VallabhPrakashan, Pitampura.
3. Foye, W.O., Lemke, T.L., William, D.A. *Principles of Medicinal Chemistry*, (4th Ed.), New Delhi. ND: B.I. Waverly Pvt. Ltd.
4. El-Mansi, E.M.T., Bryce, C.F.A., Ddemain, A.L., Allman, A.R., *Fermentatias microbiology and biotechnology*, (2nd Ed.), Taylor & Francis.
5. Prescott & Dunn's (2004). *Industrial Microbiology*, CBS Publisher

Suggested e-Sources:

1. National Programme on Technology Enhanced Learning
<https://nptel.ac.in>
2. Online Chemistry Courses
<https://www.edx.org/learn/chemistry>
3. Free Online Education SWAYAM
<https://swayam.gov.in>

BT 604R Renewable Energy Sources

Max. Marks : 100

L T P C

(ESA: 100)

0 0 4 2

Learning Outcomes:

After successful completion of the course, students will be able to:

- Understand the various forms of conventional and non conventional energy resources.
- Design working models of renewable energy.
- Understand the applications and limitations of renewable energy sources.

Section A

Availability, importance, utilization, economics and growth rates of renewable energy sources. Combustion calculations, Conventional thermal power plant design and its operation, Superheat, reheat and regeneration, Other auxiliaries of thermal plant. High– pressure boilers, Steam generator control. Biomass and its types, Biomass fuel characterization; thermo chemical and biochemical processes; reaction kinetics; energy and mass balance equations; studies of processes and system design for gasification, pyrolysis and liquefaction of biomass. Biochemical and thermochemical conversion of biomass. Design of biogas plants and gasifiers; Fuel related properties of biomass; planning and management of biomass collection, utilization, handling and pre-conditioning processes such as size reduction and densification; combustion, pyrolysis and gasification of biomass, photosynthetic efficiency, plant productivity and bio-energy yield, biomass waste.

Section B

Chemistry, process and performance analysis of biofuels; alcohol production: pre-treatment of biomass, fermentation with process details and dehydration; operational performance of I.C. engines on producer gas, biogas, alcohol, and plant oils and their esters. Solar radiation intensity and solar geometry. Analysis and design of non-concentrating and concentrating solar collectors. Solar energy storage techniques, Steady and transient heat transfer analysis of solar cookers, solar ponds, solar stills and solar dryers.

Design of solar thermal systems; hot water systems, space heating and cooling systems, solar drying system for agricultural produce etc. Economic analysis of solar energy systems. Design of solar energy operated systems for heating, cooling, distillation, drying, dehydration, water pump and power generation for applications in agriculture.

Section C

Basic principles of wind energy conversion, site selection considerations, classification advantages and disadvantages of Wind Energy Conversion System (WECS), types of wind machines, performance of wind machines, Utilization of wind energy for generating electricity and mechanical power. Types of wind mill and their characteristics. Mechanics of wind mills. Introduction to geothermal energy and storage, hydrothermal resources, geo-pressured resources, petro-thermal resources, prime movers for geothermal energy conversion, applications of geothermal energy. Basic principle of tidal power, components of tidal power plant, site requirements, storage of tidal energy, advantages and limitations of tidal power generation. Photo-Voltaic devices. Applications of renewable energy sources.

Recommended Books:

- Ching T. Hou and Jei Fu Shaw, Biocatalysis and Bioenergy, John Wiley & Sons, 2008.
- G.D. Rai, Non-Conventional Energy Sources, Khanna Publishers.
- Godfrey Boyle, Renewable Energy, Power for a Sustainable Future, Oxford University Press, U.K, 1996.
- H. P. Garg, J. Prakash, Solar Energy: Fundamentals and Applications: Fundamentals and Applications 1 Edition, Tata Mcgraw Hill Education Private Limited (2000).
- Johnson Gary, L., Wind Energy Systems, Prentice Hall, New York, 1985.
- L.L. Freris, Wind Energy Conversion systems, Prentice Hall, UK, 1990.

BIO 602R Bioethics, Biosafety and IPR

Max. Marks : 100

L T P C

(ESA: 100)

0 0 4 2

Learning Outcomes:

After successful completion of the course, students should be able to:

- Explain role of biotechnology in sustainable research and various ethical implications.
- Understand biosafety–objective, implementation, necessity and legislations.
- Develop preliminary understanding of Intellectual Property with emphasis on patents.

Section A

History and principles of bioethics, ethical dimensions of medicine and biotechnology viz. organ transplant, human genome project, cloning, surrogacy, artificial insemination, egg donation abortion, euthanasia.

Convention on biological diversity; Overview of Cartagena Protocol, Codex Alimentarius, FAO, OECD and their role in enforcing Biosafety; Role of NGOs in biotechnology.

Section B

Issues of Biosafety; Introduction to Biological Safety Cabinets; Primary Containment for Biohazards; Biosafety Levels; Recommended Biosafety Levels for Infectious Agents and Infected Animals; Biosafety guidelines - Government of India; Roles of Institutional Biosafety Committee, RCGM, GEAC etc. for GMO applications in food and agriculture; Environmental release of GMOs; Biosafety management

Section C

History of IPR, types of IPR; Role of WIPO and WTO in IPR.

Classification of patents; granting of patents and patenting authorities; rights and duties of patent owner; Patent infringement- meaning, scope and litigation; Invention in context of “prior art”; Patent databases; Country-wise patent searches (USPTO, EPO, India etc.).

US Patent act; Indian Patent act. Filing of a patent application; Precautions before patenting-disclosure/non-disclosure; WIPO Treaties; Budapest Treaty; PCT and Implications; Role of a Country Patent Office; Case studies in IPR.

Suggested Readings:

1. Bioethics and Biosafety by M.K. Sateesh. I.K. International
2. Biosafety and bioethics. Ed. Raj Mohan Joshi. Isha Books
3. Bioethics. An introduction to the history, methods and practice. By N. Jecker, A.R. Jonsen and R.A. Perlman. Jones and Bartlett publications
4. and Bioethics by Deepa Goel and Shomini Parashar. Pearson
5. [http:// Bioethics by S. Ignacimuthu s.j. Narosa Publishing House Pvt. Ltd.](#)
6. IPR, Biosafety www.w3.org/IPR/
7. <http://www.wipo.int/portal/index.html.en>
8. http://www.ipr.co.uk/IP_conventions/patent_cooperation_treaty.html
9. www.patentoffice.nic.in
10. www.iprlawindia.org/ - 31k - Cached - Similar page
11. <http://www.cbd.int/biosafety/background.shtml>
12. <http://www.cdc.gov/OD/ohs/symp5/jyrtext.html>
13. <http://web.princeton.edu/sites/ehs/biosafety/biosafetypage/section3.html>

Online Reading Elective

ICT in Teaching and Learning

Learning Outcomes:

On completion of course, the students will be able to:

- use learning assistance for learning and teaching.
- develop new teaching and learning methods, techniques and tools.

Introduction of ICT, emerging views in using ICT, teacher directed learning and learner directed learning, roles and functions of e-tutor in online teaching and learning, benefits of ICT in teaching learning and educational management, smart classroom for content delivery, web-cast lecture delivery, techniques for various learning mode, open educational resources, integration of open educational resource, virtual lab, videos, interactive video tutorial and virtual reality in teaching and learning, integration of OER in research, integration of individualized, blended and flipped learning in teaching and learning.

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