DEPARTMENT OF APPLIED CHEMISTRY

Scheme of Examination and Syllabus for the Five-Year Integrated M.Sc. Chemistry

(From 2024 admission onwards)

Approved by the Combined Board of Studies in Physical and Mathematical Sciences and Chemical and Biological Sciences on 4th April 2024

Cochin University of Science and Technology
Kochi-22

Preamble

Department of Applied Chemistry was established in 1976 with the support of UGC. Throughout the last few decades, the Department has continued to instill a scientific spirit in the students and impart strong basic theoretical and experimental skills to students. The department has always been keen to pave the path for high-quality education ensuring best career opportunities for the students. The Department is steadfast in its resolve to inculcate a spirit of continuous learning and social skills in the students, to kindle creative ideas and to equip them to face the future challenges in an enthusiastic manner.

The 5-Year Integrated M.Sc. Chemistry offered by the Department of Applied Chemistry is a trans-disciplinary non-professional course designed with an outcome-based syllabus which ensures that the students assimilate the subject in totality and can take it to further levels of application and creativity wherever required. The syllabus offers a flexibility of programme structure while ensuring that students get a strong foundation and gains indepth knowledge in chemistry. The first three Semesters provide an opportunity to cover the fundamentals in different science disciplines depending on the interests of students. From the fourth semester the students will undergo specialized courses in chemistry. The programme emphasizes the development of practical and analytical skills in students. The curriculum offers wide opportunities to specialize in their respective areas of interest along with acquiring practical skills. An entire semester dedicated to project work in institutes of national repute ensures wide scientific exposure to students and evokes research interest in advanced topics of current relevance.

Program Outcomes: Integrated M.Sc.

PO 1: Demonstrate a comprehensive understanding of fundamental principles and concepts in basic sciences.

PO 2: Analyse, evaluate, and synthesize complex scientific information and data using appropriate methods and techniques.

PO 3: Apply scientific reasoning and critical thinking adeptly to recognize, assess, and resolve problems encountered in various scientific and technological contexts.

PO 4: Utilize computational power, programming languages, and modern technologies proficiently to address scientific challenges, effectively integrating technological solutions into problem-solving processes.

PO 5: Achieve proficiency in using modern scientific tools and technologies for experimentation, data collection, analysis, and interpretation.

PO 6: Adhere to ethical principles and practices in the conduct of scientific research and professional activities, and work collaboratively with others.

PO 7: Engage in lifelong learning and professional development to enhance the knowledge and skills in basic sciences.

Program Specific Outcomes: Integrated M.Sc Chemistry

PSO 1: Acquire a systematic and coherent awareness of fundamentals and its applications in problem solving, and analytical and critical rationalizations.

PSO 2: Attain a firm grip on the basic and advanced principles of experimental/instrumental methods of analysis, and to execute them suitably for an in-depth analysis of chemical problems..

PSO 3: Acquire skills to design and perform scientific experiments and to accurately record and analyze the experimental results.

PSO 4: Acquire overall core competency in the subject and acquire skills for employment in academia and industry.

PSO 5: Acquire knowledge relevant to cater to the needs of present day society in the local/national/global arena.

PSO 6: Impart research and professional skills to undertake academia/industrial assignments by inculcating the spirit of team work, innovation and entrepreneurship

Academic pathways offered by Department of Applied Chemistry

Chemistry Major:

3-year UG Program: To earn a Chemistry Major in a 3-year UG Program, a student must complete a minimum of 68 credits in Chemistry, out of which 60 credits shall be from mandatory core courses (DSC) and 8 credits from elective (DSE) courses.

4-year UG Program (Honours): To earn a Chemistry Major in a 4-year UG Program (Honours), a student must complete a minimum of 104 credits in Chemistry, out of which 84 credits shall be from DSC courses and 16 credits from DSE courses and 4 credits from mini project.

4-year UG Program (Honours with Research): To earn a Chemistry Major in a 4-year UG Program (Honours with Research), a student must complete a minimum of 104 credits in Chemistry, out of which 84 credits shall be from DSC courses and 8 credits from DSE courses and 12 credits from a research project.

Chemistry Minor:

3-year UG Program: To earn a Minor in Chemistry in a 3-year UG Program, a student must complete a minimum of 27 credits in Chemistry, out of which 24 credits shall be from DSC courses and 03 credits from an SEC elective.

4-year UG Program: To earn a Minor in Chemistry in a 4-year UG Program, a student must complete a minimum of 35 credits in Chemistry, out of which 24 credits shall be from mandatory DSC courses, 3 credits from an SEC elective 8 credits from DSE courses.

Discipline mention in Chemistry:

To earn a Discipline mention in Chemistry in a UG Program (3 or 4 years), a student must complete a minimum of 12 credits in Chemistry from DSC courses.

Semester -wise Scheme

Semester I

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours /week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0101	Introduction to Atomic Structure, Bonding and Quantitative Analysis	100	Chemistry Major -DSC Chemistry Minor -DSC Chemistry Disci - DSC	4	3-0-2	50	50	100
24-808-0102	Chemistry in Everyday Life	100	Chemistry Minor-DSC	4	4-0-0	50	50	100
24-808-0103	General Chemistry -I	100	MDC	3	3-0-0	50	50	100
Semester Credits for Chemistry Major	21 (AEC: 6, MDC: 3, Major pathway: 4, Minor pathway: 8) Cumulative credits: 21							

L: Lecture, T: Tutorial, P: Practical

Chemistry Major-DSC: Core course for students Majoring in Chemistry.
Chemistry Minor-DSC: Core course for students Minoring in Chemistry.
Chemistry Disci-DSC: Core course for students who choose discipline mention in Chemistry.
Chemistry -MDC: Multidisciplinary elective course offered to students whose Major or Minor pathways are different from Chemistry.
AEC: Ability Enhancement Course (Languages). MDC: Multidisciplinary Course.

Semester II

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours/ week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0201	Introduction to Physical Chemistry and Inorganic Qualitative Analysis	100	Chemistry Major -DSC Chemistry Minor-DSC Chemistry Disci-DSC	4	3-0-2	50	50	100
24-808-0202	Electrochemistry, Solid State and Colloids	100	Chemistry Minor -DSC	4	4-0-0	50	50	100
24-808-0203	General Chemistry II	100	Chemistry MDC	3	3-0-0	50	50	100
Semester Credits for Chemistry Major	21 (AEC: 6, MDC: 3, Major pathway: 4, Minor pathway: 8) Cumulative credits: 42							

Semester III

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours/ week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0301	Introduction to Organic Chemistry and Organic Qualitative Analysis	100	Chemistry Major -DSC, Chemistry Minor-DSC, Chemistry Disci-DSC	4	3-0-2	50	50	100
24-808-0302	Elements of symmetry and Spectroscopy	200	Chemistry Minor-DSC	4	4-0-0	50	50	100
24-808-0303	General Chemistry III	100	Chemistry MDC	3	3-0-0	50	50	100
Semester Credits for Chemistry Major	21 (VAC: 6, MDC: 3, Major pathway: 4, Minor pathway: 8) Cumulative credits: 63							

Semester IV

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours /week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0401	Inorganic Chemistry I	200	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0402	Organic Chemistry I	200	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0403	Physical Chemistry I	200	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0404	Theoretical Chemistry I	200	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-04YY*	SEC -I	200	Chemistry SEC	3	2-0-2	50	50	100
Semester Credits for Chemistry Major	22 (VAC: 3, SEC: 3, Major pathway: 16) Cumulative credits: 85							

* Skill Enhancement Course

Semester V

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours /week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0501	Inorganic Chemistry II	300	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0502	Organic Chemistry II	300	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0503	Physical Chemistry III	300	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0504	Theoretical Chemistry II	300	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0505	Advanced Organic Synthesis and Industrial Chemistry Lab	300	Chemistry Major -DSC	4	0-0-8	100	-	100
24-808-05YY	SEC II	300	Chemistry -SEC	3	1-0-4/ 2-0-2	50	50	100
Semester Credits for Chemistry Major		23 (SEC: 3, Major pathway: 20) Cumulative credits: 108						

Semester VI

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours/ week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0601	Inorganic Chemistry III	300	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0602	Organic Chemistry III	300	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0603	Physical Chemistry III	300	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0604	Advanced Physical and Inorganic Chemistry Lab	300	Chemistry Major -DSC	4	0-0-8	100	-	100
24-808-06XX	Elective I*	300	Chemistry Major -DSE Chemistry Minor -DSE	4	4-0-0	50	50	100
24-808-06YY	SEC III	300	Chemistry SEC Chemistry Minor – DSE	3	1-0-4	50	50	100
Semester Credits for Chemistry Major		23 (SEC: 3, Major pathway: 20) Cumulative credits: 131						

* Elective courses for Chemistry Major/Minor

Internship

Students have to complete an internship of 2 credits (60 Hours of work) before the beginning of Semester VII. Cumulative Credits: 133

Exit with 3-year UG Degree OR continue to the 4th year.

Semester VII

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours /week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0701	Inorganic Chemistry IV	400	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0702	Organic Chemistry IV	400	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0703	Theoretical Chemistry III	400	Chemistry Major -DSC	4	3-0-2	50	50	100
24-808-0704	Scientific Writing and Presentation	500	Chemistry Major -DSC	2	0-0-4	100	-	100
24-808-07XX	Elective II	400	Chemistry Major -DSC Chemistry Minor– DSE	4	4-0-0	50	50	100
24-808-07XX	Elective III	400	Chemistry Major -DSE Chemistry Minor-DSE	4	4-0-0	50	50	100
Semester Credits for Chemistry Major	22 (Major/ minor pathway: 22) Cumulative credits: 155							

Semester VIII

For Honours with Research

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours /week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0801	Research Proposal Writing	500	Chemistry Major -DSC	2	1-0-2	100	-	100
24-808-0802	Project	500	Chemistry Major -DSC	12	0-0-24	200	100	300
24-808-0803	Advanced Analytical and Instrumentation Techniques	500	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0804	MOOC	400	Chemistry Major -DSE	4			100	100
Semester Credits for Chemistry Major	22 (Major and Minor pathway: 22) Cumulative credits: 177							

For Honours

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours /week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0801	Research Proposal Writing	500	Chemistry Major -DSC	2	1-0-2	100	-	100
24-808-0802	Mini Project	500	Chemistry Major -DSC	4	0-0-8	50	50	100
24-808-0803	Advanced Analytical and Instrumentation Techniques I	500	Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0804	MOOC	400	Chemistry Major -DSE	4				100
24-808-08XX	Elective IV	400	Chemistry Major -DSE Chemistry Minor -DSE	4	4-0-0	50	50	100
24-808-08XX	Elective V	400	Chemistry Major -DSE Chemistry Minor -DSE	4	4-0-0	50	50	100
Semester Credits for Chemistry Major	22 (Major and pathway: 22) Cumulative credits: 177							

Exit with 4-year UG Degree (177 Credits) OR continue to the 5th year.

Semester IX

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours /week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-0901	Advanced Analytical and Instrumentation Techniques II		Chemistry Major -DSC	4	4-0-0	50	50	100
24-808-0902	Advanced Instrumentation Lab	600	Chemistry Major -DSC	4	0-0-8	100	-	100
24-808-0903	Mini Project	600	Chemistry Major -DSC	4	0-0-8	50	50	100
24-808-09XX	Elective VI	500	Chemistry Major -DSE	4	4-0-0	50	50	100
24-808-09XX	Elective VII	500	Chemistry Major -DSE	4	4-0-0	50	50	100
Semester Credits for Chemistry Major	20 (Major pathway: 20) Cumulative credits: 197							

Semester X

Course Code	Course Name	Level	The course can be taken towards obtaining credits for:	Credits	Hours/ week L-T-P	Marks distribution		
						CA	ESE	Total
24-808-1001	Major Project	600	Chemistry Major -DSC	20	0-0-40	600		600
24-808-1002	MOOC **	500	Chemistry Major -DSE	4			100	100
Semester Credits for Chemistry Major	22 (Major pathway: 24) Cumulative credits: 221							

**Department Council will approve a set of courses the students can take. Students can take one MOOC course with 4 credits or 2 courses with 2 credits depending on the availability to complete the credit requirements. The students can enroll for the courses during IXth semester and the credits will be added to the Xth semester grades. If a students fails a course, he/she may take same or another course with the approval of the Department council.

LIST OF SKILL ENHANCEMENT COURSES

SEC I

24-808-0405 Industrial Chemistry

SEC II

24-808-0506 Advanced Techniques in Organic Synthesis: Theory and Practice

24-808-0507 Spectro Analytical Chemistry

SEC III

24-808-0605 Visualization and Computing

LIST OF ELECTIVES

ELECTIVE I

24-808-0605

24-808-0606

ELECTIVE II, III

24-808-0705 Polymer Chemistry

24-808-0706 Supramolecular Chemistry

ELECTIVE IV,V

24-808-0805 Electronic Structure From Molecules to Solids

24-808-0806 Advanced Organic Chemistry I

24-808-0807 Material Chemistry

24-808-0808 Transition Metals: Chemistry and applications in Organic Synthesis

ELECTIVE VI, VII

24-808-0904 Computational Materials Chemistry

24-808-0905 Advanced Organic Chemistry II

Syllabus

24-808-0101 Introduction to Atomic structure, Bonding and Quantitative Analysis 4 (4 Credits)

LTP 3-0-2 Level: 100
Pre-requisite: None

CO	CO Statement	CL
CO1	Appreciate the evolution of quantum mechanics and correlate the concepts to modern atomic structure.	Apply
CO2	Analyse the structure and bonding in simple molecules by applying the concepts of MOT.	Analyse
CO3	Correlate the physical and chemical properties of elements based on their periodic classification.	Apply
CO4	Perform a statistical analysis of experimental data	Apply
CO5	Quantitative estimation through titrimetric analysis	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	1	1	0
CO2	2	2	1	1	1	0
CO3	2	2	3	2	1	0
CO4	2	2	2	1	1	0
CO5	1	1	1	1	2	1

Module I (11 hrs)
Atomic structure I - Blackbody emission and temperature, Photoelectric effect, Double slit experiment, Line spectrum of elements, Rutherford's experiment, Bohr's atomic model, Failure of Classical mechanics, Evolution of quantum mechanics - Heisenberg's uncertainty principle and its significance, wave particle duality, de Broglie equation.

Module II (11 hrs)
Atomic Structure -II - Quantum atomic model, hydrogen atomic orbitals and quantum numbers, atomic orbital equations (no derivation required), Sign of wave functions. Radial and angular wave functions. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Contour boundary and probability diagrams.

Module III (12 hrs)
Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Lande equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Solvation energy, Covalent bond, Valence Bond theory, Resonance and resonance energy, Molecular orbital theory. bonding, non- bonding, antibonding molecular orbitals (concept only) elementary pictorial approach of homo- and hetero-diatomic molecules H_2, B_2, C_2, O_2, N_2, CO, NO and CO_2, H_2O etc.

Module IV (11 hrs)
Periodic Properties: Atomic weights, Development of periodic law, The modern periodic table, Basis of periodic classification, orbital types and periodic table, Commonality in electronic configurations,

Atomic sizes, ionization energy, Electronegativity, Electron Affinity, Polarizability and polarizing power, Relative orbital energies and overlap, Trends associated with properties – Physical and chemical, Anomalies in periodic properties.

Module V (Lab 30 hrs)

Titrimetric analysis and calculations: Different types of titrations - neutralization, redox (permanganometry, dichrometry, iodometry, iodimetry), complexometric (EDTA titrations) and precipitation titrations.

Principle of all types of titrations, titration curves, indicators. Significant figures, Accuracy, Precision, Error, Types of errors- Determinate and Indeterminate errors, Distribution of random errors, Mathematical Expression for error- Absolute and Relative error, Methods to reduce error, Statistical tools for expressing precision- Standard deviation, Relative standard deviation, Variance, Comparison of results- Student's t test, f test, Criteria for rejecting a value-Q test, Confidence interval

Recommended Books

1. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
2. Housecroft, C. and Sharpe, G., Inorganic Chemistry, 4th Edn., Pearson, 2012.
3. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Edn., Oxford Press, 2006
4. Lee, J.D. Concise Inorganic Chemistry, 5th Edn., John Wiley & Sons, 1999.
5. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, 3rd Ed., Oxford, 1994.
6. Day, M.C. and Selbin,J. Theoretical Inorganic Chemistry, 2nd Edn., ACS Publications, 2002.
7. Skoog, West, Holler, Crouch, Fundamentals of Analytical Chemistry, Wiley, 9th Edn.
8. Fifield, F. W., Kealey, D., Principles and Practice of Analytical Chemistry, Academic Press, 5th Edn.
9. Robinson, J. W., Skelly Frame, E. M., Frame, G. M., II, Undergraduate Instrumental Analysis, Prentice Hall, 2009
10. Vogel's Textbook of Quantitative Chemical Analysis, 6th Edn, ELBS, 1998.

24-808-0102 Chemistry in Everyday Life (4 Credits)

L-T-P 4-0-0 Level:100
Pre-requisite: None

CO	CO Statement	CL
CO1	Understand the importance and the role of chemistry in everyday life	Understand
CO2	Learn about chemicals that lay the foundation for life	Understand
CO3	Understand the type of chemicals used in household activities, cosmetics and medicine	Apply
CO4	Apply knowledge of chemistry to improve quality of life	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	1	2	0	1	1
CO2	3	1	2	1	2	0
CO3	2	2	3	2	1	1
CO4	2	2	2	1	1	1

Module I (10 hrs)

Molecules of Life - Cellular and chemical foundations of life, water unique properties, Carbohydrates and their sources, monosaccharides and disaccharides, examples, Lipids, Amino acids, Nucleic acids, Vitamins, Nutrients, Enzymes, Hemoglobin, structure and function, effect of CO, chlorophyll.

Module II (15 hrs)

Chemistry for food: chemicals used in kitchen, Butter and edible oils, composition, importance, properties, saturated and unsaturated fatty acids, hydrogenated oils, milk and dairy products, chemistry of cooking, chemical and physical changes during cooking, microwave cooking, nutrients and their stability during cooking, food preservation, colouring and flavouring agents, Beverages, food adulteration, food poisoning.

Module III (10 hrs)

Chemistry for cleaning: Soaps, chemical composition, preparation, cleaning action, synthetic detergents, bleaching, other house hold cleaning agents, tooth paste, mouth wash, sanitizers, shaving cream, shampoo disinfectants and antiseptics

Module IV (10 hrs)

Chemistry for cosmetics: Basic concepts-composition and classification, Skin chemistry, deodorants, antiperspirants, perfumes fragrances, effect of sunlight on skin, vitamin D, skin burns, sun screens, skin and hair care products, talcum powder, lipstick, moisturizers, colouring and bleaching agents, cosmetic formulations, baby care products

Module V (15 hrs)

Chemistry for medicines: Contribution of chemistry to human health and historical developments in medicine, Classification and nomenclature, Structure and function of: Analgesics – aspirin, paracetamol, Anthelmintic drug: mebendazole, Antiallergic drug: Chlorpheniramine maleate, Antibiotics: Penicillin V, Chloromycetin, Streptomycin. Sulfa drugs, Anti-inflammatory agent: Oxypheno-butazone, Antimalarials: Primazuine phosphate & Chloroquine, tranquilizer, antidepressants, antihistamines, drugs for chemotherapy, Generic and brand names

Recommended Text Books:

1. Chemistry in Daily Life by KIRPAL SINGH, PHI Learning Pvt Ltd
2. Chemistry Connection, The Chemical Basis of Everyday Phenomena, Karukstis, Kerry K. and Van Hecke, Gerald R, Harcourt/Academic Press (2003)
3. Chemistry in the Marketplace (5th ed.) Harcourt Brace (1998)
4. Introduction to Industrial Chemistry, B. K. Sharma: Goel Publishing, Meerut (1998)
5. Medicinal Chemistry by Asthoush Kar
6. Drugs and Pharmaceutical Sciences Series, Marcel Dekker, Vol.II, INC, New York.
7. Foods – Facts and Principles. N. Shakuntala Many and S. Swamy, 4th ed. New Age International (1998).

24-808-0103 General Chemistry -1 (3 Credits)

L-T-P 3-0-0 Level: 100

Pre-requisite: None

CO	CO Statement	CL
CO1	Appreciate the evolution of quantum mechanics and correlate the concepts to modern atomic structure.	Apply
CO2	Analyse the structure and bonding in simple molecules by applying the concepts of MOT.	Analyse
CO3	Correlate the physical and chemical properties of elements based on their periodic classification.	Apply
CO4	Perform a statistical analysis of experimental data	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	1	1	0
CO2	2	2	1	1	1	0
CO3	2	2	3	2	1	0
CO4	2	2	2	1	1	0

Module I (11 hrs)

Atomic structure I - Blackbody emission and temperature, Photoelectric effect, Double slit experiment, Line spectrum of elements, Rutherford's experiment, Bohr's atomic model, Failure of Classical mechanics, Evolution of quantum mechanics - Heisenberg's uncertainty principle and its significance, wave particle duality, de Broglie equation.

Module II (11 hrs)

Atomic Structure -II - Quantum atomic model, hydrogen atomic orbitals and quantum numbers, atomic orbital equations (no derivation required), Sign of wave functions. Radial and angular wave functions. Radial and angular distribution curves. Shapes of s, p, d and f orbitals. Contour boundary and probability diagrams.

Module III (12 hrs)

Ionic bond: General characteristics, types of ions, size effects, radius ratio rule and its limitations. Packing of ions in crystals. Born-Lande equation with derivation and importance of Kapustinskii expression for lattice energy. Madelung constant, Solvation energy, Covalent bond, Valence Bond theory, Resonance and resonance energy, Molecular orbital theory. bonding, non- bonding, antibonding molecular orbitals (concept only) elementary pictorial approach of homo- and hetero-diatomic molecules H_2, B_2, C_2, O_2, N_2, CO, NO and CO_2, H_2O etc.

Module IV (11 hrs)

Periodic Properties: Atomic weights, Development of periodic law, The modern periodic table, Basis of periodic classification, orbital types and periodic table, Commonality in electronic configurations, Atomic sizes, ionization energy, Electronegativity, Electron Affinity, Polarizability and polarizing power, Relative orbital energies and overlap, Trends associated with properties – Physical and chemical, Anomalies in periodic properties.

Acid Base concepts: Theories of acids and bases- Arrhenius Theory, Bronsted-Lowry definition, pH, PKa , PKb, Lux Flood Definition, Solvent system definition, Lewis Definition, Usanovich Definition,

Recommended Books

1. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
2. Housecroft, C. and Sharpe, G., Inorganic Chemistry, 4th Edn., Pearson, 2012.
3. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Edn., Oxford Press, 2006
4. Lee, J.D. Concise Inorganic Chemistry, 5th Edn., John Wiley & Sons, 1999.
5. Douglas, B.E. and Mc Daniel, D.H., Concepts & Models of Inorganic Chemistry, 3rd Ed., Oxford, 1994.
6. Day, M.C. and Selbin,J. Theoretical Inorganic Chemistry, 2nd Edn., ACS Publications, 2002.
7. Skoog, West, Holler, Crouch, Fundamentals of Analytical Chemistry, Wiley, 9th Edn.
8. Fifield, F. W., Kealey, D., Principles and Practice of Analytical Chemistry, Academic Press, 5th Edn.
9. Robinson, J. W., Skelly Frame, E. M., Frame, G. M., II, Undergraduate Instrumental Analysis, Prentice Hall, 2009
10. Vogel's Textbook of Quantitative Chemical Analysis, 6th Edn, ELBS, 1998

24-808-0201 Introduction to Physical Chemistry and Inorganic Qualitative Analysis (4 Credits)

L-T-P 3-0-2 Level: 100

Pre-requisite: None

CO	CO Statement	CL
CO1	Differentiate the properties of real gases from those of a perfect gas and predict the properties	Apply
CO2	Predict changes in thermodynamic parameters during a process and predict the spontaneity.	Analyse
CO3	Apply the concepts of chemical kinetics and photochemistry to calculate rate/ rate constants/quantum yield of different types of reactions	Apply
CO4	Understand the basic surface phenomena and extended application to adsorption.	Apply
CO5	Understand the basic principles of qualitative inorganic analysis and to identify the cations and anions in a given solution	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	1	1	0
CO2	3	3	2	1	1	0
CO3	3	2	2	1	1	0
CO4	3	2	2	1	1	0
CO5	3	3	3	1	1	0

Module I (11 hrs)

Gaseous State: Kinetic Theory of gases, Maxwell Boltzmann distribution of molecular velocities (Qualitative approach), Different types of velocities, Gas Laws, Ideal gas equation, Real gases- Deviation from ideal behavior- Compressibility factor, Van der Waals equation, Virial equation, PV isotherms, Continuity of states, Law of corresponding states, Critical phenomena and critical constants. Transport properties.

Module II (12 hrs)

Thermodynamics: State functions, Reversible and irreversible processes, Isothermal and adiabatic processes, First, second and third laws of thermodynamics, Concepts of work, heat, Internal energy, enthalpy, Heat capacity, entropy, Gibbs energy, Helmholtz energy, Work done in isothermal and adiabatic reversible and irreversible processes, Entropy and free energy as criteria for spontaneity and equilibrium, Unattainability of absolute zero. Standard states. Entropy and free energy changes during isothermal and adiabatic processes, Changes in entropy and free energy with Temperature and pressure, Gibbs Helmholtz equation, Maxwells relations,

Joule Thomson effect- Inversion temperature, Application of J.T effect - Liquefaction of gases.

Module III (12 hrs)

Chemical Kinetics: Rate laws, Order and molecularity, Zero, first, second and third order reactions-

Integration of rate equations, Half-life period, Arrhenius equation. Theories of Reaction rate- Collision Theory, Transition state theory (elementary concepts), Unimolecular reactions- Lindemann mechanism. Complex Reactions -Consecutive, Parallel and Opposing reactions (elementary concepts), Steady state approximation. Chain reactions, Branched chain reactions (basic concepts)
Photochemistry: Photochemical laws, Beer-Lambert Law, Quantum yield, Photophysical and photochemical processes- Jablonski Diagram, Fluorescence, Phosphorescence-, Chemiluminescence, Bioluminescence, Photosensitisation.

Module IV (9 hrs)

Surfaces and Interfaces: Surface free energy and Surface tension, Contact angles and Wetting, Surface films. capillarity, vapour pressure of droplets. Kelvin equation. pressure difference across curved surface -Laplace equation, Surface wetting- hydrophilicity and hydrophobicity.
Adsorption: Physical and chemical adsorption, adsorption isotherms- Langmuir (kinetic derivation), Freundlich and BET (No derivation) isotherms, Determination of surface area using Langmuir and BET isotherms, Catalysis- Homogeneous and heterogeneous, Enzyme catalysis.
Acid Base concepts: Theories of acids and bases- Arrhenius Theory, Bronsted-Lowry definition, pH, PKa , PKb, Lux Flood Definition, Solvent system definition, Lewis Definition, Usanovich Definition,
Generalised concepts: Ionic product of water, Common ion effect, Solubility product, Acid strength, Degree of hydrolysis of salts, Buffer solutions, Mechanism of buffer action, Henderson equation.

Module V (Lab 30 hrs)

Systematic qualitative analysis of mixtures containing two acid and two basic radicals from the list given below by semi micro method
Pb^{2+}, Cu^{2+}, Bi^{2+}, Cd^{2+}, Fe^{2+}, Fe^{3+}, Al^{3+}, Zn^{2+}, Mn^{2+}, Co^{2+}, Ni^{2+}, Ca^{2+}, Sr^{2+}, Ba^{2+}, Mg^{2+}, NH_4^{+},
CO_3^{2-}, SO_4^{2-}, NO_3^{-}, F^{-}, Cl^{-}, $C_2O_4^{2-}$, CH_3COO^{-}, PO_4^{3-}

Recommended Books

1. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10^{th}/11^{th} edn, 2017/2018.
2. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6^{th} edn (Indian) 2011.
3. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4^{th} edn, 2004.
4. T. Engel and P. Reid, Physical Chemistry, Pearson, 3^{rd} Edn, 2013.
5. K J Laidler, J.H Meiser, Physical Chemistry, 4^{th} edn 2003.
6. K. J. Laidler, Chemical-Kinetics, Paperback Edn., 2018.
7. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.

24-808-0202 ELECTROCHEMISTRY, SOLID STATE AND COLLOIDS (4 Credits)
L-T-P 4-0-0 Level: 100
Pre-requisite: None

CO	CO Statement	CL
CO1	Describe the theories of ionic conductance and apply the concepts to calculate conductance of a given system	Apply
CO2	Describe the mechanism of electronic conductance at charged interfaces.	Apply
CO3	Describe the regular arrangement of atoms in crystals and the symmetry of their arrangement	Analyse
CO4	Explain the properties of solids and correlate their mechanical, electrical, optical, and magnetic properties with their constituent atoms and molecules.	Analyse
CO5	Describe various types of colloids, their stability and properties	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	1	3	2	1
CO2	3	3	1	3	2	1
CO3	3	3	1	3	3	2
CO4	3	3	1	3	3	2
CO5	3	3	1	3	3	2

Module I (12 hours)

Introduction- Ionics, Electrodics, Electrochemical Cells, Electrodes, Electrolytes, Half Reactions, Electrochemical Work, Equilibrium electrochemistry-Half- reactions and electrodes, Types of cells, Types of electrodes- Standard hydrogen electrode, Calomel electrode, Quinhydrone electrode. Ion – Solvent, Ion – Ion Interactions, Ionic and Electronic Conductance, Conductance Measurement, Equivalent Conductance, Kohlrausch's Law, Ostwalds dilution law, Ionic Mobility, Walden's rule, abnormal conductance, Conductometeric titrations.

Module II (12 hours)

Transport Number- Factors Influencing, measurement- Hittorf's and moving boundary methods. Debye-Huckel Theory, Ionic Atmosphere, time of Relaxation, Mechanism of Electrolytic Conductance, Debye Huckel Onsager equation for strong electrolytes. Electrode – Ion interface, liquid junction potential, Double Layer, Overvoltage (Elementary idea)

The electromotive force, Standard potentials, Applications of standard potentials, Determination of solubility product and activity coefficient, pH determination, Potentiometric titrations, Redox indicators principle. Activity and Activity Coefficient of Electrolytes. Corrosion of metals- different forms of corrosion and prevention. Electrochemical Theory of corrosion – methods of prevention. Fuel Cell, Batteries (Elementary idea)

Module III (12 hours)

Crystal structures and symmetry, Crystallographic point groups, space group, unit cells, Miller indices, Seven crystal systems and Bravais lattices, Simple, body centered and face centered systems, Packing in solids- packing diagrams, close packing,- hcp and ccp structures, XRD, Braggs equation – derivation, Powder and rotating crystal technique. Identification of cubic crystals based on interplanar ratio

Module IV (14 hours)

Ionic solids with formula MX (CsCl, NaCl, Zinc Blende and Wurtzite Structures), MX2 (Fluorite and Antfluorite Structures, Cadmium Halides, CaF2, Rutile, Anti-rutile, betacristobalite), other crystal systems (Bismuth tri-iodide, Corundum, Rhenium Trioxide etc.), Mixed oxides (Spinel, Perovskite, Ilmenite). The properties of solids**,** Mechanical properties Electrical properties, Impact on nanoscience: Nanowires, Optical properties, Magnetic properties.

Point Defects in crystals- stoichiometric and non-stoichiometric defects, Line defect, surface defects, Liquid Crystals- Classification and application

Module V (10 hours)

Colloids: Lyophilic and Lyophobic colloids, Preparation of colloids, Kinetic, optical and electrical properties, Electrical double layer Models for double layer: Helmholtz, Gouy- Chapman and Stern models, Zeta potential. Stability of colloids, Protective colloids- Gold number, Flocculation, Hardy Schulze rule, Surfactants, micelles, Donnan membrane equilibrium, Dorn effect, Sedimentation potential and streaming potential, Emulsions, Gels, Sols.

Recommended Books:

1. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Edn., Wiley, New York, 1998
2. R. Crow, Principles and Applications of Electrochemistry, , 4th edn, 1994.
3. S. Glasstone, An Introduction to Electrochemistry, Paperback edn., 2007
4. L.V. Azaroff, Introduction to Solids, McGraw Hill, 1960.
5. A. R. West, Solid State Chemistry, Wiley Student (Indian) Ed., (2014)
6. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967. 35
7. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995
8. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.
9. C. N. R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry. 2nd edn, Cambridge Uty Press, 1997.
10. P.W. Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10th/11th edn, 2017/2018

24-808-0203 General Chemistry II (3 Credits)

L-T-P 3-0-0 Level: 100
Pre-requisite: None

CO	CO Statement	CL
CO1	Differentiate the properties of real gases from those of a perfect gas and predict the properties	Apply
CO2	Predict changes in thermodynamic parameters during a process and predict the spontaneity.	Analyse
CO3	Apply the concepts of chemical kinetics and photochemistry to calculate rate/ rate constants/quantum yield of different types of reactions	Apply
CO4	Understand the basic surface phenomena and extended application to adsorption.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	1	1	0
CO2	3	3	2	1	1	0
CO3	3	2	2	1	1	0
CO4	3	2	2	1	1	0

Module I (11 hrs)
Gaseous State: Kinetic Theory of gases, Maxwell Boltzmann distribution of molecular velocities (Qualitative approach), Different types of velocities, Gas Laws, Ideal gas equation, Real gases- Deviation from ideal behavior- Compressibility factor, Van der Waals equation, Virial equation, PV isotherms, Continuity of states, Law of corresponding states, Critical phenomena and critical constants. Transport properties.

Module II (12 hrs)
Thermodynamics: State functions, Reversible and irreversible processes, Isothermal and adiabatic processes, First, second and third laws of thermodynamics, Concepts of work, heat, Internal energy, enthalpy, Heat capacity, entropy, Gibbs energy, Helmholtz energy, Work done in isothermal and adiabatic reversible and irreversible processes, Entropy and free energy as criteria for spontaneity and equilibrium, Unattainability of absolute zero. Standard states. Entropy and free energy changes during isothermal and adiabatic processes, Changes in entropy and free energy with Temperature and pressure, Gibbs Helmholtz equation, Maxwells relations,
Joule Thomson effect- Inversion temperature, Application of J.T effect - Liquefaction of gases.

Module III (12 hrs)
Chemical Kinetics: Rate laws, Order and molecularity, Zero, first, second and third order reactions- Integration of rate equations, Half-life period, Arrhenius equation. Theories of Reaction rate- Collision Theory, Transition state theory (elementary concepts), Unimolecular reactions- Lindemann mechanism. Complex Reactions -Consecutive, Parallel and Opposing reactions (elementary concepts),

Steady state approximation. Chain reactions, Branched chain reactions (basic concepts)
Photochemistry: Photochemical laws, Beer-Lambert Law, Quantum yield, Photophysical and photochemical processes- Jablonski Diagram, Fluorescence, Phosphorescence-, Chemiluminescence, Bioluminescence, Photosensitisation.

Module V (9 hrs)

Surfaces and Interfaces: Surface free energy and Surface tension, Contact angles and Wetting, Surface films. capillarity, vapour pressure of droplets. Kelvin equation. pressure difference across curved surface -Laplace equation, Surface wetting- hydrophilicity and hydrophobicity.
Adsorption: Physical and chemical adsorption, adsorption isotherms- Langmuir (kinetic derivation), Freundlich and BET (No derivation) isotherms, Determination of surface area using Langmuir and BET isotherms, Catalysis- Homogeneous and heterogeneous, Enzyme catalysis.

Recommended Books

1. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, 10^{th}/11^{th} edn, 2017/2018.
2. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6^{th} edn (Indian) 2011.
3. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4^{th} edn, 2004.
4. T. Engel and P. Reid, Physical Chemistry, Pearson, 3^{rd} Edn, 2013.
5. K J Laidler, J.H Meiser, Physical Chemistry, 4^{th} edn 2003.
6. K. J. Laidler, Chemical-Kinetics, Paperback Edn., 2018.
7. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.

24-808-0301 Introduction to Organic Chemistry and Organic Qualitative Analysis (4 Credits)

L-T-P 3-0-2 Level: 100
Pre-requisite: None

CO	CO Statement	CL
CO1	Assign the nomenclature of simple organic molecules following IUPAC rules and identify various functional groups in organic chemistry.	Apply
CO2	Apply the concepts of isomerism and analyse the conformation and configuration of organic molecules.	Apply
CO3	Describe the different types of organic reactions.	Understand
CO4	Understand the different chemical bonding in organic molecules and reactive intermediates.	Understand
CO5	Understand the nature of biomolecules and develop an insight into the importance of organic chemistry in life.	Understand

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	1	1	1	1
CO2	2	3	1	1	1	1
CO3	2	3	3	2	1	1
CO4	2	2	2	1	1	1
CO5	1	2	1	1	2	1

Module I (10 hrs)

Localized and delocalized chemical bonding, the concept of aromaticity, writing proper Lewis structures, hybridization, reactive intermediates (carbynes, carbenes, carbocation, carbanion, radicals, arynes, nitrenes), Geometry of organic molecules.. "Symbolism" in Organic Chemistry.

Module II (30 hrs)

Nomenclature and functional groups in organic molecules: Rules of IUPAC system of nomenclature, naming of common organic compounds. Introduction to organic functional groups- alcohols, ethers, halides, amines, nitro compounds.

Organic Qualitative Analysis Lab

Identification of simple organic compounds.

Preparation of derivatives.

Module III (10 hrs)

Stereochemistry: Configuration and conformation- Concept of configuration, classification of stereoisomers, optical isomerism, chirality, wedge formula, Fischer projection, Newman projection, perspective formula. Relative and absolute configurations, sequence rules, D & L, R & S systems of nomenclature. Enantiomers, meso form, diastereoisomers, epimers, anomers. Geometrical

Isomerism: E-Z notation. Conformational analysis: Strain in molecules, acyclic molecules, cyclohexane, substituted cyclohexanes- A values.

Module IV (10 hrs)

Basics of reaction mechanism: Classification and an overview of organic reactions. Electron pushing diagrams. Basics of reaction coordinate diagrams, intermediates, transition states, exothermic and endothermic reactions, activation energy, rates of reactions and rate-determining step. Aliphatic Nucleophilic substitutions - SN1, SN2, substitutions on aromatic carbon, Addition reactions - polar and nonpolar addition - addition of Bromine and hydrogen halides to double bonds - Markownikoff's rule and peroxide effect., Elimination - E1, E2, E1CB, pyrolytic elimination.

Module V (15 hrs)

Introduction to carbohydrates: General introduction to carbohydrates, ring-chain tautomerism, glycosidic linkage, classification, monosaccharides, disaccharides, oligosaccharides, polysaccharides, reducing and nonreducing sugars, structure of aldohexoses, fructose and ribose, "sugar-like" artificial sweeteners, basic introduction to amino acids, proteins and nucleic acids.

Recommended Text Books

1. J. G. Smith, Organic Chemistry, 3rd edn., 2011.
2. Clayden J., Greeves, N. Warren, S., Organic Chemistry, 2nd edn. Oxford University Press, 2001.
3. Bruice, P.Y. Organic Chemistry, 7th edn., Prentice Hall Inc., 2013.
4. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th edn., Wiley, 2013.
5. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th edn., Springer, 2008.
6. J. McMurry, Organic Chemistry, 5th edn., Brooks/Cole, 2000.
7. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th edn., Prentice Hall, 1986.
8. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2 nd Ed., 2007.
9. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3 rd Ed., Viswanathan, 1957.
10. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5 th Ed., Longman, 1989

24-808-0302 Elements of Symmetry and Spectroscopy (4 Credits)

L-T-P 4-0-0 Level: 100

Pre-requisite: None

CO	CO Statement	CL
CO1	Analyze the symmetry of any given molecule and assign the point group	Analyse
CO2	Explain the principles of rotational, vibrational, Raman, electronic, fluorescence and NMR spectroscopic techniques	Understand
CO3	Predict the applications and uses of the spectroscopic techniques	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	1	3	2	1
CO2	3	3	1	3	2	1
CO3	3	3	1	3	3	2

Module I (10 hrs.)

Symmetry as a universal theme. Different symmetry classes and symmetry operations (discussion with suitable examples). Applications of symmetry to a) Polar molecules b) chiral molecules. Symmetry properties of orbitals (basic concepts); concept of point groups, identification of molecular point groups in some simple molecules.

Module II (8 hrs.)

Spectroscopy and its importance in chemistry. Link between spectroscopy and quantum chemistry. Electromagnetic radiation and its interaction with matter. origin of linewidths in molecular spectra, Transition dipole moment and Fermi's Golden Rule, Einsteins Coefficients, Lasers and Masers; Types of spectroscopy. Difference between atomic and molecular spectra. Separation of molecular energies into translational, rotational, vibrational and electronic components. Born-Oppenheimer approximation, Postulates of quantum mechanics, quantum mechanical operators.

Module III (16 hrs.)

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

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

Raman spectroscopy: Qualitative treatment of Rotational Raman effect; Effect of nuclear spin, Vibrational Raman spectra, Stokes and anti-Stokes lines; their intensity difference, rule of mutual exclusion.

Module IV (12 hrs.)

Electronic Spectroscopy: Electronic excited states. Free Electron model, its application to electronic spectra of polyenes. Franck-Condon principle, electronic transitions, Beer Lambert's Law, singlet and triplet states, fluorescence and phosphorescence, dissociation and predissociation, calculation of electronic transitions of polyenes using free electron model. Colour and constitution, chromophores, auxochromes, bathochromic and hypsochromic shifts.

Module V (14 hrs.)

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin–Spin coupling and coupling constant; Anisotropic effects, Interpretation of NMR spectra of simple compounds. Carbon-13 NMR, introduction to polarization transfer and NOE, 2D NMR, MRI, Solid state NMR

Principle of fluorescence spectroscopy, Quenching of fluorescence, Mechanisms of quenching

Recommended Books:

1. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th Ed. Tata McGraw-Hill: New Delhi, 2006.

2. W.Kemp, Organic Spectroscopy, 3rd Ed., Palgrave, 1991.

3. G. M. Barrow, Physical Chemistry, 6th Ed., McGraw-Hill College, 1996.

4. P.W. Atkins and J.Paula, Physical Chemistry, 8th Ed., Oxford Press, 2006.

5 .I. N. Levine, Physical Chemistry, 6th Ed., McGraw-Hill Education, 2008.

6. F. A. Cotton, Chemical Applications of Group Theory, 3rd Ed., Wiley Interscience, New York, 2008.

7. M. S. Gopinathan and V. Ramkrishnan, Group Theory in Chemistry, 2nd Ed., Vishal Publishing Co., 2013.

8. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley, 2005.

24-808-0303 General Chemistry III (3 Credits)

L-T-P 3-0-0 Level: 100
Pre-requisite: None

CO	CO Statement	CL
CO1	Assign the nomenclature of simple organic molecules following IUPAC rules	Apply
CO2	Apply the concepts of isomerism and analyse the conformation and configuration of organic molecules.	Apply
CO3	Describe the different types of organic reactions.	Understand
CO4	Understand the different chemical bonding in organic molecules and reactive intermediates.	Understand
CO5	Understand the nature of biomolecules and develop an insight into the importance of organic chemistry in life.	Understand

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	1	1	1	1
CO2	2	3	1	1	1	1
CO3	2	3	3	2	1	1
CO4	2	2	2	1	1	1
CO5	1	2	1	1	2	1

Module I (10 hrs)
Localized and delocalized chemical bonding, the concept of aromaticity, writing proper Lewis structures, hybridization, reactive intermediates (carbynes, carbenes, carbocation, carbanion, radicals, arynes, nitrenes), Geometry of organic molecules.. "Symbolism" in Organic Chemistry.

Module II (7 hrs)
Nomenclature and functional groups in organic molecules: Rules of IUPAC system of nomenclature, naming of common organic compounds. Introduction to organic functional groups- alcohols, ethers, halides, amines, nitro compounds.

Module III (10 hrs)
Stereochemistry: Configuration and conformation- Concept of configuration, classification of stereoisomers, optical isomerism, chirality, wedge formula, Fischer projection, Newman projection, perspective formula. Relative and absolute configurations, sequence rules, D & L, R & S systems of nomenclature. Enantiomers, meso form, diastereoisomers, epimers, anomers. Geometrical Isomerism: E-Z notation. Conformational analysis: Strain in molecules, acyclic molecules, cyclohexane, substituted cyclohexanes- A values.

Module IV (8 hrs)
Basics of reaction mechanism: Classification and an overview of organic reactions. Electron pushing diagrams. Basics of reaction coordinate diagrams, intermediates, transition states, exothermic and

endothermic reactions, activation energy, rates of reactions and rate-determining step. Aliphatic Nucleophilic substitutions - SN1, SN2, substitutions on aromatic carbon, Addition reactions - polar and nonpolar addition - addition of Bromine and hydrogen halides to double bonds - Markownikoff's rule and peroxide effect., Elimination - E1, E2, E1CB, pyrolytic elimination.

Module V (10 hrs)

Introduction to carbohydrates: General introduction to carbohydrates, ring-chain tautomerism, glycosidic linkage, classification, monosaccharides, disaccharides, oligosaccharides, polysaccharides, reducing and nonreducing sugars, structure of aldohexoses, fructose and ribose, "sugar-like" artificial sweeteners, basic introduction to amino acids, proteins and nucleic acids.

Recommended Text Books

1. J. G. Smith, Organic Chemistry, 3rd edn., 2011.
2. Clayden J., Greeves, N. Warren, S., Organic Chemistry, 2nd edn. Oxford University Press, 2001.
3. Bruice, P.Y. Organic Chemistry, 7th edn., Prentice Hall Inc., 2013.
4. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th edn., Wiley, 2013.
5. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th edn., Springer, 2008.
6. J. McMurry, Organic Chemistry, 5th edn., Brooks/Cole, 2000.
7. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th edn., Prentice Hall, 1986.
8. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2 nd Ed., 2007.
9. Dey, B.B. Sitaraman, M.V. and Govindachari, T.V. Laboratory Manual of Organic Chemistry, 3 rd Ed., Viswanathan, 1957.
10. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5 th Ed., Longman, 1989

24-808-0401 INORGANIC CHEMISTRY I: Inorganic Main Group and Nuclear Chemistry (4 Credits)

L-T-P 4-0-0

Pre-requisite: 24-808-0101 or equivalent

CO	CO Statement	CL
CO1	Interpret the types of bonding and structure based on the electronic configuration	Apply
CO2	Explain the reactivity and physicochemical properties based on the type of bonding	Analyse
CO3	Explain the properties of transition metals and lanthanides	Apply
CO4	Compare the structure, bonding and reactivity of the compounds of main group elements	Analyse
CO5	Describe the radioactivity phenomena and its applications	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	2	1	0
CO2	2	2	1	2	1	0
CO3	2	2	1	2	1	0
CO4	2	2	1	2	1	1
CO5	2	2	1	2	1	1

Module I (10 hrs)

s- Block elements- Hydrogen, Hydrogen Bonding, Hydrates, Hydrogen ions, acids and bases,

Group 1 elements - General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Flame colors and spectra, Color of compounds, Alkali metals in liquid ammonia and other solvents, Oxides, hydroxides, hydrides, alkoxides, amido complexes, Ionic salts and M^+ ions in solution, Alkali metal complexes, Organolithium compounds.

Module II (10 hrs)

Group 2 elements – General Behavior, Occurrence and abundance, Electronic Configuration and types of bonding, Elemental Beryllium, Binary Compounds, Coordination compounds with oxygen and nitrogen ligand, organoberyllium compounds, Compounds of Magnesium, Calcium, Strontium-oxides, halides, hydrides, carbides, ionic salts and complexes, alkoxides. Grignard reagents – preparation and properties.

Module III (14 hrs)

General periodic trends of d and f block elements, Metallic property, Chemistry of variable oxidation states, properties of d configuration - d^0 to d^{10}, Type of compounds. physical and chemical

properties of transition elements; Difference between first row and other rows, Double salts and coordination compounds.

Introduction to coordination compounds; coordination numbers and geometries in transition metal complexes; nomenclature; isomerism in transition metal complexes – structural, geometrical and optical isomerism.

Lanthanides and Actinides- Stable oxidation states, lanthanide and actinide contraction, Occurrence and recovery; Separation of Lanthanides; difference between 4f and 5f orbitals, Industrial importance of lanthanides.

Actinides: Comparison with lanthanides and general characteristics

Module IV (14 hrs)

Types of oxides, Chemical properties of Dioxygen, Singlet oxygen, ozone, Peroxo compounds, Superoxide. Nitrogen compounds- Nitrides, Ammonia, Hydrazine, Oxides of Nitrogen, Oxo acids and anions.

Sulphur-Nitrogen compounds: Tetrasulphur tetranitride, disulphur dinitride and polythiazyl. SxNy compounds. S-N cations and anions. Sulphur-phosphorus compounds: Molecular sulphides such as P4S3, P4S7, P4S9 and P4S10. Phosphorus-nitrogen compounds: Phosphazenes and poly phosphazenes.

Interhalogen compounds, Structure, hybridization and reactivity of ClF3, ICl3, IF5 and IF7, Compounds of Xe, Kr and Rn.

Module V (12 hrs)

Nuclear radius, Nuclear Forces, Nuclear Spin, Magnetic dipole moment, Elementary Particles, Binding Energy, Nuclear models – Shell model- magic number, periodicity in nuclear properties, Liquid drop model – Fission and Fusion, Nuclear Stability, Exchange theory, n/p ratio, Nuclear Radiations, Nuclear reactions, Types of nuclear reactions, Decay Kinetics, Half-life, Radioactive disintegration series. Fission: Fission products and Fission yield curve, Fission energy, theory of nuclear fission, nuclear reactor, breeder reactor - nuclear reactors in India. Fusion reactions, hydrogen bomb and energy of sun. Radio carbon dating principles.

Recommended Text Books:

1. Mingos, D. M. P., Essential Trends in Inorganic Chemistry, Oxford University Press 1998.
2. Wulfsberg G., Inorganic Chemistry, VIVA, 2002.
3. Greenwood, N. N., Earnshaw, A., Chemistry of the Elements, Maxwell Macmillan International Edition, Pergamon Press, 1989.
4. Cotton, F.A., Wilkinson, G, Advanced Inorganic Chemistry. Wiley-VCH, 1999
5. Huheey, J. E., Keiter, E. A., Kieter, R. L., Medhi, O. K., Inorganic Chemistry Principles Structure and Reactivity, Pearson Education, 4th edition, 2009.
6. Lee, J. D., A New Concise Inorganic Chemistry, ELBS, 1998
7. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
8. Arnikar, H. J., Essentials of Nuclear Chemistry, Wiley Eastern Ltd., New Delhi, 1982.

24-808-0402 Organic Chemistry I: Stereochemistry, Reaction Mechanisms & Rearrangements (4 Credits)

L-T-P 4-0-0 Level: 200

Pre-requisite: 24-808-0301 or equivalent

CO	CO Statement	CL
CO1	Apply the concepts of isomerism and analyze the conformation and configuration of organic molecules.	Apply
CO2	Illustrate the mechanism involved in various reactions.	Apply
CO3	Describe bonding properties in organic molecules.	Understand
CO4	Illustrate the mechanistic pathway of different rearrangement reactions and identify the products	Apply
CO5	Predict the reactivity of an organic compound based on its structure and the reaction conditions	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	1	2	3	1	1
CO2	1	1	2	3	1	1
CO3	1	1	2	3	1	1
CO4	1	1	3	3	1	1
CO5	2	2	3	3	1	1

Module I (12 hrs)

Stereochemistry: Geometrical & Optical isomerism: the origin of chirality, chiral centres and configuration, axes and planes, helicity. Prochiral centres and faces. Topicity relationships, enantiotopic and diastereotopic groups and faces. Symmetry, stereochemistry and time scale. Allenes, cumulenes, biphenyls, and spirans. Compounds containing chiral atoms other than carbon.

Conformational analysis: Acyclic molecules, cyclohexane, substituted cyclohexanes- A values.

Strain, types of strain including B, F, I, Pitzer strain and Baeyer strain. Acyclic sp^3–sp^3, sp^3-sp^2 systems, structure and stability of small, medium, and large rings, cyclohexane, substituted cyclohexanes, cyclohexenes, decalins, and bicyclic systems. Kinetic vs thermodynamic control in ring forming reactions.

Module II (14 hrs)

The study of reactions and the methods of studying reaction mechanisms:– Classification of reactions according to IUPAC conventions. Reaction mechanism: guidelines on Pushing of electrons. Reactive intermediates: Formation, stability and general reactivity. Methods of determining reaction mechanisms (kinetic and non-kinetic methods): The Hammond postulate, reactivity vs selectivity principle, the Curtin-Hammett principle, microscopic reversibility, kinetic *vs* thermodynamic control. Isotope effects: Primary, secondary and Equilibrium isotope effects, Tunneling effects, solvent isotope effects, and heavy atom Isotope effects.

Linear free energy relationships: Hammett and Taft parameters, Solvent effects (Grunwald-Winstein plots and Schleyer adaptation), nucleophilicity and nucleofugality. Isokinetic and Isoequilibrium temperature, Enthalpy – entropy compensation. Experimental techniques to determine reaction

mechanisms: identification of intermediates by trapping and competition experiments, cross-over experiments, isotope scrambling, radical clocks and traps, matrix isolation.

Module III (14 hrs)

Substitutions on Aliphatic carbon: –saturated and unsaturated systems – Mechanism of nucleophilic substitution – S_N2, S_N1 – ion pairs, SET, Neighbouring group participation – non-classical carbocations, SNi, Tetrahedral mechanism. Electrophilic substitution – SE2, SEi, SE1. Free radical substitution. Reactivity – Effect of substrate structure, nature of reagents, solvents and stereochemistry on the outcome of these reactions. Ambident nucleophiles and substrates. Typical reactions involving substitution.

Substitutions on aromatic carbon: Mechanism of electrophilic, nucleophilic and free radical substitutions – orientation and reactivity. Typical reactions involving aromatic substitution.

Module IV (10 hrs)

Additions and eliminations:

Mechanisms of polar addition – electrophilic, nucleophilic and free radical addition. Nonpolar additions (excluding pericyclic reactions) - Reactivity and orientation.

Eliminations - E2, E1 and E1CB mechanisms, reactivity and orientation. Pyrolytic syn eliminations, α - eliminations, elimination *vs* substitution. Typical reactions involving addition and elimination.

Module V (10 hrs)

Rearrangements: Wagner-Meerwein, Pinacol, Demyanov, dienone-phenol, Favorskii, Wolff, Hofmann, Curtius, Lossen, Schmidt, Beckmann, benzidine, and Hofmann-Loffler, Fries, Baeyer-Villiger rearrangements. Fritsch-Buttenberg-Wiechell rearrangement, Corey-Fuchs reaction, Wittig rearrangement.

Recommended Text Books

1. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
2. March, J., Smith, D., March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th ed., Wiley, 2013.
3. Bruice, P.Y. Organic Chemistry, 7th ed., Prentice Hall Inc., 2013.
4. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
5. J. McMurry, Organic Chemistry, 5th ed., Brooks/Cole, 2000.
6. P. Sykes, Guidebook to Mechanism in Organic Chemistry, 6th ed., Prentice Hall, 1986.
7. E. L. Eliel and S. H. Wilen, Stereochemistry in Organic Compounds, John Wiley, 1994.
8. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 10th ed., New Age Publications, 2019.
9. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.

24-808-0403 Physical Chemistry I: Equilibrium and Statistical and Irreversible Thermodynamics (4 Credits)

L-T-P 4-0-0 Level: 200

Pre-requisite: 24-808-0201 or equivalent

CO	CO Statement	CL
CO1	Predict the dependence of physical and chemical equilibrium on pressure, temperature and concentration.	Apply
CO2	Apply the concept of chemical potential in physical and chemical processes.	Apply
CO3	Understand the thermodynamics of phase transitions and interpret the phase diagram of a given system	Analyse
CO4	Apply the principles of statistical thermodynamics to ideal gases, solids and metals.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	2	1	1	0
CO2	3	3	2	1	1	0
CO3	3	3	3	1	1	0
CO4	3	2	2	1	1	0

Module I (11 hrs)

Recap of the laws of thermodynamics and thermodynamic functions.

Thermochemistry- Enthalpy of physical and chemical changes, Temperature dependence of reaction enthalpies, Hess's law.

Chemical Equilibria: Chemical Equilibria and free energy, Equilibrium Constant, Applications of free energy function to physical and chemical changes- Le Chateliers Principle. Effect of temperature and pressure on the chemical equilibrium- van't Hoff reaction isotherm and isochore.

Module II (11 hrs)

Thermodynamics of Mixtures: Partial molar quantities, Chemical potential, Thermodynamics of mixing, Excess function, Chemical potential of liquids, Gibbs Duhem Equation and Duhem Margules Equation. Ideal solutions, Deviations from ideality, Concepts of fugacity and activity, Ideal dilute solutions, Henry's and Raoult's laws, Colligative properties, Regular solutions.

Module III (11 hrs)

Physical Transformation of substances: Phase stability and transitions, phase equilibria of pure substances, Clausius Clapeyron equation, Solid-liquid, liquid-vapor and solid-vapor equilibria, phase rule, phase diagrams of one-component systems, Ehrenfest Classification of Phase transitions.

Phase Equilibria of Binary and ternary Systems: Vapor pressure-composition diagrams, Temperature-composition diagrams, Liquid-liquid systems – Completely miscible, Partially miscible and Immiscible, Azeotropes and Azeotropic distillation, Steam distillation. Solid-Liquid systems, Solid-vapour systems.

Three-component systems.

Module IV (15 hrs)

Thermodynamic probability, microstate and macrostate, entropy and probability, most probable distribution, residual entropy and its calculation. Ensembles, Maxwell - Boltzman statistics.

Quantum statistics: Bose - Einstein statistics, Fermi - Dirac statistics, Comparison of Maxwell - Boltzman, Bose- Einstein and Fermi - Dirac Statistics, Dilute Systems.

Partition function and its relation to thermodynamic properties: Translational, rotational and Vibrational partition function. Molecular partition function for delocalized systems, calculation of equilibrium constant using partition functions. Heat capacity of gases and solids. Anomalous heat capacity of hydrogen.

Module V (12 hrs)

Linear Non-equilibrium thermodynamics: General theory, Local entropy production, balance equation for concentration. Energy conservation in open systems. Entropy balance equation. Forces and Fluxes, Steady state and local equilibrium conditions. Linear phenomenological laws. Phenomenological coefficient, Systems with heat, matter and electrical transport, Onsager Reciprocal relation, Application to Diffusion -Thermal diffusion, Thermal Osmosis and electrokinetic effects, Soret Coefficient, Seebeck effect.

Recommended Books

1. P.W Atkins, Julio De Paula, Physical Chemistry, Oxford University Press, $10^{th}/11^{th}$ edn, 2017/2018.
2. Ira.N.Levine, Physical Chemistry, Tata Mc Graw Hill, 6^{th} edn (Indian) 2011.
3. R.A.Alberty & R.J.Silbey, Physical Chemistry, Wiley Publishers, 4^{th} edn, 2004.
4. D.A McQuarrie, J.D Simon, Molecular Thermodynamics, Viva Student Edn. 2010.
5. L. K. Nash, Elements of Chemical Thermodynamics, Addison Wesley, 2^{nd} Edn, 2013.
6. F.W Sears, Introductions to Thermodynamics, Kinetic Theory of Gases and Statistical Mechanics, Addision Wesley Pub. Cambridge, 1998.
7. F.C. Andrews, Equilibrium to Statistical Mechanics, John Wiley, New York, 2002.
8. L.K. Nash, Statistical Thermodynamics, Addison Wesley, New York, 1999.
9. D. A. McQuarrie, Physical Chemistry- A Molecular Approach, South Asian Edn., 2008.
10. D. A. McQuarrie, Statistical Thermodynamics, South Asian Edn., 2008.
11. M. Dole, Introduction to Statistical Thermodynamics, Prentice Hall, London, 1997.

24-808-0404 Theoretical Chemistry I: Quantum Mechanics (4 Credits)

L-T-P 4-0-0 Level: 200

Pre-requisite: None

CO	CO Statement After the completion of the course the student will be able to	CL
CO1	Describe and justify the importance of Quantum Mechanics	Analyse
CO2	Understand and apply various postulates in deriving property operators and Schrodinger equation	Apply
CO3	Apply the postulates of quantum mechanics to simple systems of chemical interest, such as the particle-in-a-box, harmonic oscillator, rigid rotor and Hydrogen atom	Analyse
CO4	Interpret the solutions and appreciate the quantization concept	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	1	0	2	1	0
CO2	3	1	0	2	1	0
CO3	3	1	0	3	1	0
CO4	3	2	0	3	2	1

Module I (15 hrs)

Basics: Evolution of quantum mechanics, Heisenberg's matrix mechanics- commutator relationships, position representation, coordinate- Cartesian, cylindrical and spherical polar and their interconversion, Complex number and their representation in various coordinate systems. Operators, Algebra of operators, Linear and Hermitian operators, Eigenvalue equation, Significance, well-behaved functions, Time dependent Schrodinger equation, conservative and non-conservative systems

Module II (10 hrs)

Solving the Schrodinger equation-Particle in a box: Quantum mechanical postulates, construction of various operators – kinetic energy, angular momentum. Translational motion- free particle, particle in one, two and three-dimensional box (rectangular and cubical), separation of variables, concept of degeneracy, introduction to quantum mechanical tunneling.

Module III (12 hrs)

Solving the Schrodinger equation-Simple Harmonic oscillator: Vibrational motion, 1-D Harmonic oscillator, Method of power series, Hermite equation and Hermite Polynomials, Recursion formula, wave function and energy. Transition moment integral, selection rules, Extension of the results to 3D-SHO.

Module IV (08 hrs)

Solving the Schrodinger equation-Planar Rigid Rotor: Rigid rotator, Conversion of laplacian opertor into spherical polar coordinates, Particle on a ring, phi equation, Angular momentum operator L^2 and Lz, quantization, polar plots. Solving the Schrodinger equation-Non-planar RR: Theta equation and solutions Lagendre equation and Lagendre polynomials, Restriction of m_l values, Spherical harmonics,Angular momentum operator L^2 and Lz, Space quantization, polar plots of spherical harmonics.

Module V (15 hrs)

Solving the Schrodinger equation- iv) Hydrogen atom: Separation into three equations and solutions, Theta and phi equations and solutions, Spherical harmonics, Radial equations and solutions, Laguerre equation and Laguerre polynomials. Solutions of wave functions and energies, quantum numbers and their importance, Radial wave function and radial distribution functions, angular wave function, Shapes of s, p, d and f atomic orbitals.

Recommended Text Books:

1. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Ed., Oxford Press, 2006.
2. Szabo, A.; Ostlund, N. S. “Modern Quantum Chemistry: Introduction to Advanced Electronic Structure theory”, Dover Publications, 1996.
3. Levine, I. N. "Quantum Chemistry", 7th Ed., Pearson Education Inc., 2014.
4. McQuarrie, D. A., "Quantum Chemistry", 2nd Ed.,University Science Books, 2008.
5. Pillar, F. L. “Elementary Quantum Chemistry”, 2nd Ed., Dover Publication, 2001.
6. Chandra, A. K., "Introduction to Quantum Mechanics", 4th Ed, Tata McGraw-Hill, New Delhi, 2003.
7. Prasad, R. K., “Quantum Chemistry”, 4th Ed, New Age International, 2009.

24-808-0405 Industrial Chemistry (3 Credits)

L-T-P 2-0-2 Level: 200

Pre-requisite: None

CO	CO Statement	CL
CO1	Prepare and analyze industrially important chemical products	Create
CO2	Prepare the treatment methods for conversion of natural resources to value added chemicals	Create

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	1	2	2	3	3
CO2	2	1	2	2	2	3

Module 1 (15 hours)

Fats and oils general introduction, chemical composition of fats and oils, quality parameters, sources and classification, value added products from vegetable oils. Cleaning products general introduction, Chemistry of cleaning action, classification of cleaning products, Soap and Detergents, chemical composition, principles of preparation, different methods, builders and additives, quality parameters Margarine- Importance, chemical composition, preparation methods, principles of emulsification Biodiesel: energy scenario, consumption pattern, fossil fuel depletion and environmental issues, Alternate solutions, transesterification; FT process, catalysts; biodiesel purification, fuel properties

Module 2 (8 hours)

Water purification: Concept of Pure Water, Water Contamination, Water Purification Methods, Water quality parameters

Module 3 (7 hours)

General introduction to essential oils and natural flavours, natural sources, extraction techniques and principles

Module 4 (10 hours)

Practice: Preparation, characterization and quality analysis of value added products from vegetable oils (soap, margarine, vanaspati

Module 5: (10 hours)

Practice: Purification of contaminated water, estimation of quality parameters, pH, conductivity, Total Dissolved Solids, hardness, turbidity, Dissolved oxygen, COD, chloride

Module 6: (10 hours)

Practice: Extraction and characterization of essential oils and flavours from natural sources

Recommended Text Books:

1. Krishna Chattopadhyay and Manas Mandal ANALYTICAL CHEMISTRY SKILL ENHANCEMENT COURSE, CBSCBS Publishers & Distributors, 2022
2. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan,

2014.
3. J. B. Yadav, Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016

24-808-0501 INORGANIC CHEMISTRY-II: Polyhedral Boranes, Coordination & Bioinorganic Chemistry and (4 Credits)

L-T-P 4-0-0 Level: 300
Pre-requisite: 24-808-0401 or equivalent

CO	CO Statement	CL
CO1	Describe and explain the structure, bonding and magnetism of metal complexes using CFT.	Analyse
CO2	Describe the metal-ligand interactions in terms of sigma and pi bonding and covalency using LFT and MO theory	Evaluate
CO3	Understand the importance of metal ions in living systems	Analyse
CO4	Predict the stability and topology of different polyhedral boranes and related compounds.	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	3	2	1
CO2	3	2	1	3	2	1
CO3	3	2	1	2	2	1
CO4	3	2	1	3	2	1

Module I (10 hrs)
Werner's theory, Effective atomic number, Bonding in coordination compounds.

Valence bond description and its limitations. valence bond theory (inner and outer orbital complexes). Crystal Field Theory (CFT). d-orbital splitting in octahedral and tetrahedral geometries, measurement of 10 Dq (Δo), crystal field stabilization energy, CFSE in weak and strong fields, effect of pairing energy, factors affecting the crystal-field parameters.

Crystal field splitting of square planar, trigonal bipyramidal, trigonal planar and linear geometries.

Module II (12 hrs)
Application of crystal filed theory, colour and spectral behaviours. magnetism of first-row transition metal complexes, lattice energies, ionic radii, site preferences in spinels. Spectrochemical series, Demerits of CFT.
Octahedral vs. tetrahedral coordination, tetragonal distortions from octahedral geometry Jahn-Teller theorem, Jahn – Teller effect in octahedral and tetrahedral complexes, square planar geometry. Stabilization of unusually low and high oxidation states of metals.

Module III (12 hrs)

Molecular Orbital Theory: construction of molecular orbital diagrams (using group theory-qualitative idea only), qualitative MO diagrams for octahedral, tetrahedral and square planar complexes, effect of π-bonding, experimental evidence for π-bonding, spectrochemical series.
Ligand field theory, Effect of π-donor and π-acceptor ligands in LFSE, back bonding.

Module IV (12 hrs)

Metal ions in biological systems - Biochemistry of iron – Haemoglobin and myoglobin - O2 and CO_2 transportation (Elementary idea of structure and oxygen binding), Structure and mechanism of action of sodium potassium pump - Biochemistry of Ca, Zn and Co – Toxicity of metal ions (Pb, Hg and As). Anticancer drugs: *Cis*-platin, oxaliplatin and carboplatin– Structure and significance.
Non-Heme Iron Proteins: Iron storage and transfer – ferritin, transferrin; electron transfer (Iron-sulfur protein) – rubredoxin, ferredoxin; O_2 transport – hemerythrin
Copper proteins and Enzymes–Hemocyanin, superoxide dismutase, ceruloplasmin, cytochrome C oxidase; Zinc and Cobalt enzymes carbonic anhydrase, carboxypeptidase, interchangeability of zinc and cobalt enzymes; Vitamin B12; Photosynthesis and N_2 fixation.

Module V (14 hrs)

Electronic structure and allotropes of boron, boron halides, boron heterocycles, borazine Structure and bonding in polyhedral boranes and carboranes, styx notation; electron count in polyhedral boranes; Wade's rule; topological approach to boron hydride structure. Importance of icosahedral framework of boron atoms in boron chemistry. Closo, nido and arachno structures. Synthesis of polyhedral boranes;
Electron counting in polycondensed polyhedral boranes, mno rule. Carboranes, metallocarboranes.

Recommended Text Books:

1. Purcell, K.F & Kotz, J.C. Inorganic Chemistry, 2nd Ed., W.B. Saunders Co, 1991.
2. Huheey, J. E., Keiter, E. A. and Keiter, R. L. Inorganic Chemistry, Principle and structure and reactivity, 4th Ed., Harper Collins College Publishers, New York, 1993.
3. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
4. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
5. Cotton, F.A. & Wilkinson, G, Advanced Inorganic Chemistry. 6th Ed., Wiley- Interscience, 1999.
6. Shriver, D. F., Atkins, P. W. and Langford, C. H. Inorganic Chemistry, 4th Ed., W.H. Freeman & Company, 2006.
7. Lippard, S.J. & Berg, J.M. Principles of Bioinorganic Chemistry 2nd Ed., University Science Books, 1994.
8. Greenwood, N.N. & Earnshaw A., Chemistry of the Elements, 2nd., Ed. Butterworth-Heinemann,1997.
9. Sharpe, A.G. Inorganic Chemistry, 4th Indian Reprint, Pearson Education, 2005.
10. Douglas, B. E.; McDaniel, D.H. and Alexander, J.J. Concepts and Models in Inorganic Chemistry 3rd Ed., John Wiley and Sons, NY, 1994.
11. W. L. Jolly, Modern Inorganic Chemistry, McGraw-Hill International, 2nd Edition, New York, 1991.

24-808-0502 Organic Chemistry II: Analytical and Spectroscopic Techniques (4 Credits)

L-T-P 4-0-0 Level: 300

Pre-requiste: None

CO	CO Statement	CL
CO1	Apply the principles of separation, purification and chromatographic techniques in organic synthesis.	Apply
CO2	Identify structures of simple organic compounds based on the data from UV-Vis, IR, Mass Spectrometry, ^{1}H NMR and ^{13}C NMR spectroscopy.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	3	3	3	1	1
CO2	2	3	3	3	1	1

Module I (12 hrs)

Separation and Purification Techniques: Recrystallization, use of drying agents, sublimation. General principles of distillation, fractional distillation, steam distillation, and distillation under reduced pressure. Solvent extraction. Chromatographic Techniques: Chromatography - Principle of differential migration. Classification of chromatographic methods. Basic principles and uses of Thin layer chromatography (TLC), Paper chromatography (PC), Rf value, Column chromatography, Gas chromatography (GC), High-performance Liquid chromatography (HPLC), and Size exclusion chromatography.

Module II (12 hrs)

UV-visible Spectroscopy: Types of electronic transitions, Chromophores and Auxochromes, Bathochromic and Hypsochromic shifts, Intensity of absorption; Effect of structure on absorption characteristics, Application of Woodward Rules for calculation of λ_{max} for the following systems: α,β-unsaturated aldehydes and ketones, λ_{max} for polyenes, aromatic aldehydes, ketones, esters.

IR spectroscopy: Fundamental and non-fundamental molecular vibrations; IR absorption positions of O and N containing functional groups; Effect of H-bonding, concentration, temperature, conjugation, resonance and ring size on IR absorptions; Fingerprint region and its significance; application in functional group analysis. Fourier transform IR, group frequencies, fundamental frequencies and overtones, combination tones, Fermi Resonance. Basic introduction to Raman spectroscopy.

Module III (14 hrs)

NMR Spectroscopy: Basic principles of Proton Magnetic Resonance, chemical shift and factors influencing it; Spin–Spin coupling and coupling constant; Anisotropic effects in alkene, alkyne, aldehydes and aromatics, Interpretation of NMR spectra of simple compounds. Proton decoupled Carbon-13 NMR, introduction to polarization transfer and NOE.

Module IV (11 hrs)

Mass spectrometry – Introduction. EI ionization. Fragmentation modes and determination of molecular mass by MS.

Soft ionization techniques, ion separation and analysis, and hyphenated techniques.
HRMS and molecular formula.

Module V (11 hrs)
Problems based on the combined application of various spectroscopic techniques.

Recommended Books

1. Brian S. Furniss, Antony J. Hannaford, Peter W. G Smith, Austin R.Tatchell, Vogel's Textbook of Practical Organic Chemistry, 5th Edition, Longman Scientific and Technical, 1989.
2. D.L.Pavia, G.M. Lampman, G.S.Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
3. R. M. Silverstein, G.C. Bassler, T. C. Morril, Spectroscopic identification of organic compounds, John Wiley, 1991.
4. D. H. Williams, I. Fleming, Spectroscopic Methods in Organic Chemistry, Tata McGraw Hill. 1988.
5. W. Kemp, Organic Spectroscopy, 2nd ed., ELBS-Macmillan, 1987.
6. Spectral databases (RIO DB of AIST, for example).
7. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, 1996.

24-808-0503 Physical Chemistry II: Chemical Kinetics, Surface Chemistry and Catalysis (4 Credits)

L-T-P 4-0-0 Level: 300

Pre-requisite: 24-808-0201 or equivalent

CO	CO Statement	CL
CO1	Interpret the basic reaction dynamics and kinetics of various reactions and obtain the rate constants for reactions in gaseous state and solutions.	Analyse
CO2	Calculate the thermodynamic parameters from kinetic data	Apply
CO3	Apply the basic principles of acid-base and enzyme catalysis to any given kinetic data.	Apply
CO4	Explain the fundamentals of photochemical and photophysical processes and energy/electron transfer.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	3	1	1	2
CO2	3	3	2	1	1	2
CO3	3	2	3	1	1	2
CO4	3	2	2	1	1	2

Module I (12 hrs)

Complex Reactions: Parallel, Consecutive and Opposing reactions, Steady state Approximation, Kinetics of chain reactions - Photochemical reactions H_2-Cl_2 and H_2-Br_2 reaction, Organic decomposition reactions-Rice Herzfield mechanism (acetaldehyde and ethane), Branched Chain Reactions, Explosions-

Somenoff Hinshelwood mechanism (H_2-O_2 reaction), Termolecular reactions.

Module II (12 hrs)

Molecular reaction dynamics: Reactive encounters, Theories of reaction rates-Collision Theory recap), Activated Complex Theory- Potential energy surface, Erying equation, Comparative evaluation of collision and transition state theory, Thermodynamic treatment of reaction rates. Theory of unimolecular reactions- Lindemann Mechanism, Modifications to Lindemann mechanism- Hinshelwood, RRK and

RRKM model. Termolecular reactions. Molecular beam methods, Stripping and rebound mechanism.

Module III (12 hrs)

Reactions in Solutions: Cage effect, Transition state theory for reactions in solutions, Effect of ionic strength, dielectric constant and Internal pressure. Primary and secondary salt effect. Solute-solvent interactions. Ion dipole and dipole-dipole reactions. Diffusion controlled reactions. Isotope effects: Equilibrium isotope effects. Primary and Secondary kinetic isotope effects

Module IV (12 hrs)

Surface Chemistry: Gibbs adsorption isotherm. BET isotherm (derivation).

Catalysis: Catalysis and Inhibition, Homogeneous and heterogeneous Catalysis – Transition state theory, General mechanism. General Mechanism of homogeneous catalysis- Arrhenius and vant Hoff intermediates, Acid base catalysis- specific and general acid catalysis, Enzyme catalysis- Michaelis- Menten Mechanism, Competitive and non competitive inhibition. Kinetics of Surface catalysis: Unimolecular and bimolecular Surface reactions. Kinetics of adsorption- Langmuir Hinshelwood mechanism and Rideal-Eley mechanism. Autocatalysis- Oscillatory reactions- Lotka- Volterra, Oregonator, Brussellator.

Module V (12 hrs)

Photochemistry: Photochemistry and photophysics- Applications, Excited state reactivity and life time, Excimers and Exciplex, Energy and electron transfer -Elementary idea, Quenching- Static and Dynamic, Stern Volmer equation, Applications- Photocatalysis and artificial photosynthesis (Elementary principles).

Recommended Text Books

1. W. J. Moore and R. G. Pearson, Kinetics and Mechanism, Wiley, New York.
2. K. J. Laidler, Chemical-Kinetics, McGraw Hill, New York.
3. M. R. Wright, An Introduction to Chemical Kinetics, Wiley, 2004.
4. Richard Masel, Chemical kinetics and Catalysis, Wiley Interscience.
5. P. W. Atkins, Physical Chemistry 8th Edn., Wiley, New York.
6. Christian Reichardt, Solvents and Solvent effects in Organic Chemistry, Wiley VCH 2003.
7. A. W. Adamson, The Physical Chemistry of Surfaces, 2nd Edn., Wiley. New York

24-808-0504 Theoretical Chemistry II: Spectroscopy (4 Credits)
L-T-P 4-0-0 Level: 300
Pre-requisite: None

CO	CO Statement	CL
CO1	Explain the factors affecting the intensity and broadening of lines in spectra and methods to enhance the sensitivity.	Understand
CO2	Explain the principles of rotational, vibrational, Raman, electronic, ,fluorescence, NMR and ESR.	Understand
CO3	Calculate the energy required for a particular type of energy transition and determine the parameters involved.	Apply
CO4	Apply various theoretical aspects to various spectroscopic techniques for prediction of different spectroscopic observations.	Analyse
CO5	Identify various d-d transitions and interpret the electronic spectra of any giventransition metal complex.	Apply
CO6	Interpret the ESR and Mossbauer spectra of given transition metal complex.	Evaluate

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	1	3	2	1
CO2	3	3	1	3	2	1
CO3	3	3	1	3	3	2
CO4	3	3	1	3	3	2
CO5	3	3	1	3	3	2
CO6	3	3	1	3	3	2

Module I (8 hours)

Population of energy levels. Induced quantum transitions. Integrated absorption coefficient. Einstein's coefficients of absorption. Basis of selection rules, transition moment integral. Beer's Law. Induced absorption and emission of radiation by molecules, Factors affecting the intensity and width of spectral lines, Methods to reduce line broadening.

Module II (14 hours)

Rotational and vibrational energies of diatomic molecules. Linear molecules, Symmetric top and asymmetric top molecules. Rotation spectra: Diatomic and polyatomic molecules, Selection rule.
Vibration spectra of diatomic molecules, Morse potential of real molecules, overtones, combination and hot bands, Fermi resonance, rotational character of vibration spectra. Coupling of rotation and vibration. Parallel and perpendicular bands.

Vibration spectra of polyatomic molecules, Normal modes of vibrations of polyatomic molecules. Raman Spectroscopy. Rotational Raman spectra. Vibrational Raman spectra, Resonance Raman, mutual exclusion principle. Selection rules and applications to IR and Raman spectra, Surface enhanced Raman spectroscopy.
Applications of Group theory for molecular vibration, symmetry of group vibrations. Selection rules and applications to IR and Raman spectra.

Module III (14 hours)
Electronic energy states of molecules. Selection rules for electronic transitions, Vibrational structure of electronic bands. Electronic transitions and absorption bands. Electronic spectra of diatomic and polyatomic molecules, its relation to electronic arrangement and symmetry of molecules. Different types of electronic transitions, Electronic spectra of conjugated systems.
Principle of fluorescence spectroscopy, Quenching of fluorescence, Mechanisms of quenching Magnetic resonance spectroscopy: Theory of nuclear magnetic resonance, Chemical shifts, Factors affecting chemical shifts, First order and second order spectra, relaxation effects. Fourier Transformation in NMR, Measurement of relaxation time, Spin echo, NOE, 2D NMR, NQR Spectroscopy. MRI, Solid state NMR.
Principle of electron spin resonance.

Module IV (12 hours)
Microstates, Atomic term symbols Free ion terms for dn configuration, Splitting of terms in octahedral and tetrahedral octahedral fields, Correlation diagram for d2 configuration in octahedral geometry, d-d transitions, Selection rules for electronic transitions.
Orgel diagram – splitting for d1, d9, high spin d4, d6, splittings for high spin d2, d3, d8 and d7. Calculation of Dq, B and β
Tanabe Sugano diagrams – splittings for low spin dn systems
Electronic Spectral interpretation of some coordination compounds
Consequence of Jahn Teller effect on the electronic spectra of coordination compounds
Charge transfer spectra, Electronic spectra of lanthanide and actinide complexes

Module V (12 hours)
Electronic paramagnetic resonance spectroscopy: Electronic Zeeman effect, Zeeman Hamiltonian and EPR transition energy. EPR spectrometers, presentation of spectra. The effects of electron Zeeman, nuclear Zeeman and electron nuclear hyperfine terms in the Hamiltonian on the energy of the hydrogen atom. Second order effect. 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.

Mossbauer spectra of Fe (II) and Fe (III) cyanides.

Recommended Text Books:

1. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
2. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann Advanced Inorganic Chemistry, 6th ed., Wiley-Interscience: New York, 1999.
3. J.E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and

Reactivity, 4th ed., Harper Collin College Publishers, 1993.

4. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
5. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., John Wiley and Sons, 1994.
6. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., BH, 1997.
7. R. S.Drago, Physical Methods for Chemists, 2nd ed., Saunders College Publishing, 1992.
8. C. E. Housecroft, A. G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.
9. W. L. Jolly, Modern Inorganic Chemistry, 2nd ed., McGraw-Hill, New York, 1991.
10. Solid state chemistry: an introduction, Lesley Smart and Elaine Moore, 4th ed. Taylor and Francis, 2012.
11. Earnshaw, A. Introduction to Magnetochemistry, Academic Press, 1968.
12. Carlin, R.L. Magnetochemistry, Spinger-Verlag, Berlin, 1986.
13. P. W. Atkins, Physical Chemistry 8th ed., W. H. Freeman, New York, 2006.
14. R. A. Alberty, Physical Chemistry 8th ed., Wiley, New York, 1994.
15. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw Hill, New York, 1962
16. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 4th ed., Tata McGraw Hill, 1996.
17. H. Gunther, NMR Spectroscopy, 2nd ed., John Wiley, 2005.

24-808-0505 Advanced Organic Synthesis And Industrial Chemistry Lab (4 Credits)
L-T-P 0-0-8 Level: 300
Pre-requisite: 24-808-0301 or equivalent

	Course Outcome	CL
CO1	Prepare organic compounds through one step synthesis and purify and recrystallize the product.	Analyse
CO2	Plan and perform synthetic procedures, chromatographic separation and purification of organic compounds.	Understand
CO3	Use software to Draw the structures and schemes of organic molecules and reactions.	Apply
CO4	Separate organic compounds from the organic binary mixture and identify the functional group(s) present.	Analysis
CO5	Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc. to search, analyse and collect chemical information.	Apply
CO6	Prepare and analyze industrially important chemical products	Create
CO7	Prepare the treatment methods for conversion of natural resources to value added chemicals	Create

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	3	3	3	3
CO2	3	3	3	3	3	3
CO3	3	3	3	3	3	3
CO4	3	3	3	3	3	3
CO5	2	3	3	3	2	3
CO6	2	3	3	2	3	3
CO7	3	3	3	3	3	3

Module I

One step synthesis of Organic Compounds, General methods of separation and purification of Organic compounds such as 1) Solvent extraction 2) Thin layer chromatography and paper chromatography 3) column chromatography.

Module II

Part I: Separation and identification of the components of organic binary mixtures.

Part II: Preparation of Organic compounds by multistep reactions. Progress of the reactions should

be followed by spectroscopic and chromatographic methods. Purification of products and characterisation using UV-Vis, FTIR and NMR.

Part III : Use Chemical Abstracts, Scopus, Organic Synthesis collective volumes on web etc., to search, analyse and collect chemical information.

Module III -V

1. Preparation of soap and detergents

2. Preparation of margarine

3. Preparation and physical property measurement of natural, synthetic rubber, fiber.

4. Extraction of essential oils

5. Extraction of natural flavors

6. Preparation of Biogas

7. Wastewater treatment

8. Preparation and characterization of nanomaterials

9. Preparation of silicon from Rice Husk

10. Galvanization/powder coating

Recommended Textbooks:

1. Pavia, D.L. Lampman, G.M. Kriz, G.S. and Engel, R.G. Introduction to Organic Laboratory Techniques: A small scale Approach, 2nd Ed., 2007.
2. Mann, F.G. Saunders, B.C. Practical Organic Chemistry, 4th Ed., Pearson Education India, 2009.
3. Furniss, B.S. Hannaford, A.J. Smith, P.WG. Tatchell, A.R. Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Longman, 1989.
4. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
5. L. W. Harwood, C. J. Moody, Experimental Organic Chemistry-Principles and Practice, Blackwell Science Publications.
6. G. Pass, H. Sutcliffe. Practical Inorganic Chemistry 2nd ed., Chapman & Hill. 1974.
7. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6th Ed., Pragati Prakashan, 2014.
8. Yadav, J. B., Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.

24-808-0506 Advanced Techniques in Organic Synthesis: Theory and Practice (3 Credits)

L-T-P 1-0-4 Level: 300

Pre-requisite: 24-808-0301 or equivalent

CO	CO Statement	CL
CO1	Independently organizing and carrying out the most sophisticated and widely used organic transformations in a safe lab setting.	Apply
CO2	Characterize simple to complex molecules using spectroscopic methods.	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	3	3	3	1
CO2	3	3	3	3	3	1

Module I (7 hrs)

General methods in organic synthesis: Condensation, substitution, cycloaddition, oxidation, and reduction. Methods for heterocycles and their important reactions**.**

Module II (8 hrs)

Advanced organic reactions: Multicomponent reactions, organo-catalysed reactions, click reactions. Cross-coupling reactions, metathesis reactions, and application in the synthesis of functional molecules and drugs.

Module III (20 hrs)

Practice : General methods of separation and purification of organic compounds such as 1) Solvent extraction 2) Thin layer chromatography and paper chromatography 3) column chromatography.
Drawing the structures of organic molecules and reaction schemes by Proprietary and open source computer software. Use Chemical Abstracts, Scopus, Scifinder etc., to search, analyse and collect chemical information.

Module IV (20 hrs)

Practice: Hands-on training in conducting reactions under an inert atmosphere and usage of Schlenk line techniques. Drying of solvents like THF, methanol and toluene. Handling of the Glove box. Green strategies such as microwave, sonochemistry, electrochemical and photochemical reactions. Training in cross-coupling reactions and olefin metathesis.

Module V (20 hrs)

Practice: Characterization of synthesized molecules using GC, LCMS, IR, NMR and HPLC techniques. Determination of specific rotation of enantiopure molecules.

Recommended Text Books

1. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
2. A. I. Vogel, A. R. Tatchell, B. S. Furnis, A. J. Hannaford, P. W. G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th ed., John Wiley, 1989.
3. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 10th ed., New Age Publications, 2019.
4. T. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2000.
5. D. L. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, A Guide for Students of Organic Chemistry, 3rd ed., Thomson. 2004.
6. J. R. Mohrig, D. G. Alberg, G. E. Hofmeister, P. F. Schatz, C. N. Hammond, Laboratory Techniques in Organic Chemistry, 4th ed., W. H. Freeman and Company, 2014.

24-808-0507 Spectro Analytical Chemistry (3 Credits)

L-T-P 2-0-2 Level 300

Pre-requisite: None

CO	CO Statement	CL
CO1	Acquire theoretical and practical knowledge in instrumentation aspects of spectroanalytical devices.	Apply
CO2	Acquire skill to independently operate the instruments.	Apply
CO3	Interpret the data and derive qualitative and quantitative analysis	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	3	3	2	2
CO2	2	3	3	2	2	2
CO3	2	2	3	3	2	1

Module I (8 hrs)

A brief introduction to analytical methods in chemistry, Qualitative analysis and quantitative analysis, applications in day to day life**.** Introduction to various spectro analytical techniques, concept of light matter interaction, Jablonski Diagram and origin of different spectroscopies.

Module II (10 hrs)

Brief theoretical introduction to colourimetry, absorption spectroscopy, fluorescence spectroscopy, vibrational spectroscopy, refractometry, polarimetry, smartphone spectroscopy

Module III (12 hrs)

Detailed Instrumentation aspects of colourimeter, UV-VIS-NIR spectrometer, Fluorimeter, IR spectrometer, Raman spectrometer, refractometer, smartphone spectrometers

Module IV (10 hrs)

Practice: Colurimetry and UV-VIS spectroscopy: hands on training on the instrument, preparation of stock solutions, verification of Beeer-Lambertz law, Estimation of unknown concentration, establish correlation between molecular structure and spectrum, smartphone spectroscopy and comparison with colorimetry and UV-VIS spectroscopy

Module V (12 hrs)

Practice: vibrational spectroscopy: hands on training on the instrument, preparation of samples, IR and Raman spectroscopic characterization of organic and inorganic samples, assignment of peaks to functional groups, spectral processing, data processing, chemometry and machine learning tools., preparation of nanomaterials of surface enhanced Raman spectroscopy, comparative study of Raman and SERS

Module VI (8 hrs)

Practice: Refractometry and Polarimetry: hands on training on the instrument, preparation of stock solutions, estimation of refractive index and optical activity, estimation of unknown concentration, analysis of food samples

Recommended Text Books

1. Krishna Chattopadhyay and Manas Mandal, ANALYTICAL CHEMISTRY SKILL ENHANCEMENT COURSE,
2. Gurtu, J. N., Gurtu, A., Advanced Physical Chemistry Experiments, 6th Ed.,Pragati Prakashan,2014.

24-808-0601 Inorganic Chemistry – III (4 Credits)

L-T-P 4-0-0 Level: 300

Pre-requisite: None

CO	CO Statement	CL
CO1	Analyze the symmetry of any given molecule and assign the point group	Analyse
CO2	Apply the principles of symmetry and group theory in structure, bonding and spectral characteristics of molecules	Apply
CO3	Identify the structure-activity relationship of simple molecules based on their qualitative molecular orbitals.	Apply
CO4	Assess the strength of various acids and bases and their reactivity.	Evaluate
CO5	Explain behavior of different non-aqueous solvent systems towards different reactions.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	3	2	1
CO2	3	2	1	3	2	2
CO3	3	2	1	3	2	1
CO4	3	2	1	3	2	1
CO5	3	2	1	3	2	1

Module I (15 hrs)

Matrix representation of symmetry operations, similarity transformation and classes, Symmetry classification of molecules into point groups (Schoenflies symbol)- Reducible and Irreducible representations - Great Orthogonality theorem and its consequences (statement only, proof not needed), Character tables, Reduction formula, construction of character tables for point groups with order ≤6-, Interpretation of character tables. Wave functions as bases for irreducible representations, Direct product.

Application of symmetry to predict polar and chiral compounds

Module II (15 hrs)

Application of Group theory to Hybridization of atomic orbitals: Construction of hybrid orbitals for AB3(planar), AB4(Td), AB5(D3h) and AB6(Oh) type of molecules.

Application of group theory to Molecular Orbital Theory: LCAO and Huckel approximations. Symmetry adapted linear combinations, Projection operators, Application of projection operators to pi-bonding in ethylene, cyclopropenyl systems, benzene and naphthalene. Application of projection operators to sigma bonding in ethylene and $PtCl_4$. Molecular orbitals for tetrahedral and octahedral molecules,

Applications of Group theory for molecular vibration, symmetry of group vibrations. Selection rules and applications to IR, Raman and electronic spectra.

Module III (10 hrs)

Qualitative molecular orbital theory, symmetry of molecular orbitals, MOs for homo and heteronuclear diatomic molecules, H_2 to F_2, HF, CO, NO, BeH_2, CO_2, H_2O, BH_3, NH_3, B_2H_6. Importance of frontier molecular orbitals, Shape, energy and reactivity of molecules.

Module IV (10 hrs)

Relative strength of acids, Pauling rules, Lewis concept, Generalized acid-base concept, Measurement of acid base strength, Lewis acid –base interactions, steric and solvation effects, acid–base anomalies, Pearson's HSAB concept, acid-base strength and hardness and softness, Symbiosis, theoretical basis of hardness and softness, electronegativity and hardness.

Module V (10 hrs)

Chemistry in non-aqueous solvents reactions in NH_3, liquid SO_2, solvent character, reactions in SO_2, acetic acid, solvent character, reactions in H_2SO_4 and some other solvents. Molten salts, Green solvent: supercritical CO_2, Ionic liquids and deep eutectic solvents.

Recommended Books

1. F. A. Cotton, Chemical Applications of Group theory, Wiley Eastern, Singapore, 2nd ed., 1992.
2. V. Ramakrishnan, M. S. Gopinathan, Group theory in Chemistry, Vishal Pub. New Delhi, 1996.
3. Alan Vincent, Molecular Symmetry and Group Theory: A Programmed Introduction to Chemical Applications, 2nd ed., Wiley, 2013.
4. Robert L. Carter, Molecular Symmetry and Group Theory, Wiley, 2009.
5. Kieran C. Molloy, Group Theory for Chemists: Fundamental Theory and Applications, 2nd edition, Woodhead publishing, 2010.
6. G.L. Miessler, P.J. Fischer, D.A. Tarr, Inorganic Chemistry, 5th ed., Pearson, 2014.
7. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of Structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
8. F. A. Cotton, G. Wilkinson, C. A, Murillo, M. Bochmann, Advanced Inorganic Chemistry, 6th ed., Wiley- Interscience: New York, 1999.
9. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.
10. B. Douglas, D. McDaniel, J. Alexander, Concepts and Models of Inorganic Chemistry, 3rd ed., Wiley, 1994.
11. N. N. Greenwood, A. Earnshaw, Chemistry of the Elements, 2nd ed., Butterworth-Heinemann, 1997.
12. C.E. Housecroft, A.G. Sharpe, Inorganic Chemistry, 5th ed., Pearson, 2018.

24-808-0602 Organic Chemistry III: Reactions, Reagents, Photochemistry & Pericyclic Reactions (4 Credits)

L-T-P 4-0-0 Level: 300

Pre-requiste: 24-808-0402 or equivalent

CO	CO Statement	CL
CO1	Interpret the differences in reactivity of various reducing, oxidizing agents, organometallic and organo-nonmetallic reagents with mechanistic illustrations.	Apply
CO2	Analyze the reagents and conditions for the synthesis of specific target molecules.	Analyse
CO3	Identify the mechanism and the product in a given reaction under photochemical conditions.	Apply
CO4	Apply the concepts of Frontier orbital theory in the study of pericyclic reactions.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	3	2	1	1
CO2	3	3	3	3	1	1
CO3	3	3	2	2	1	1
CO4	2	3	1	1	1	1

Module I (13 hrs)

Reagents for oxidation and reduction: Chromium reagents, activated DMSO, osmium tetroxide, selenium dioxide, singlet oxygen, peracids, hydrogen peroxide, periodic acid, lead tetraacetate, ozonolysis, Woodward and Prevost hydroxylation, Wacker process, Oppenauer oxidation, Sharpless, Shi and Jacobsen asymmetric epoxidations. Catalytic hydrogenations (heterogeneous-Palladium/Platinum/Rhodium and Nickel, homogeneous-Wilkinson), metal hydride reduction-$LiAlH_4$, DIBAL-H, Red-Al, $NaBH_4$ and $NaCNBH_3$. Selectrides, trialkylsilanes and trialkyl stannane. Birch reduction, hydrazine and diimide reduction. Meerwein-Ponndorf-Verley reaction, Enzymatic reduction using Baker's yeast.

Module II (13 hrs)

Synthetic applications of organometallic and organo-nonmetallic reagents: Hydroboration reactions, Sakurai allylation, Gilman's reagent, Ullmann and Glaser coupling reactions. Suzuki coupling, Sonogashira coupling, Heck reaction, Buchwald–Hartwig coupling, Negishi coupling and Stille coupling. Metathesis processes of electrophilic carbene complexes (first- and second-generation Grubbs catalyst), ROMP, Dötz reaction and methylenation of carbonyls.

Application of reagents such as NBS, DCC, DMAP, DEAD, DDQ. Phase transfer catalysts. Chemistry of Nucleophilic Heterocyclic Carbenes (NHCs), multicomponent reactions such as Ugi reaction, Passerini reaction and Biginelli reaction. Click reaction.

Module III (14 hrs)

Chemistry of carbonyl compounds: Reactivity of carbonyl groups in aldehydes, ketones, carboxylic acids, esters, acyl halides and amides. Substitution at carbonyl carbon, mechanisms of ester

hydrolysis, substitution at α-carbon, aldol and related reactions. Grignard reaction, Reformatsky reaction, Claisen, Darzen, Dieckmann, Knoevenagel and Stobbe condensations. Perkin, Prins, Mannich, Stork-enamine reactions. Conjugate additions, Michael additions and Robinson annulation. Favorskii reaction, Julia olefination, Peterson olefination. Preparation of 1,2-, 1,3-, 1,4- and 1,5-diketones from simple ketones.
Reaction with phosphorous and sulfur ylides

Module IV (8 hrs)
Photochemistry: Unimolecular and bimolecular processes in the excited states, mechanism of important photochemical reactions, Paterno-Buchi reaction, Norrish Type I and Type II fragmentation, di-pi-methane rearrangement, Barton reaction, photochemistry of olefins, arenes, cyclohexadienones; photoreduction and photo-oxygenation.

Module V (12 hrs)
Pericyclic reactions: Study of the principle of conservation of orbital symmetry: Orbital symmetry diagrams for cycloaddition and electrocyclic reactions. Aromatic Transition State Theory and The Generalized Woodward – Hoffmann rule applied to cycloadditions, Electrocyclic reactions, Sigmatropic rearrangements and Chelotropic reactions. Pericyclic Reactions in Organic Synthesis: Stereochemistry and Regiochemistry of Cycloadditions. Substituent and medium effects, Secondary Orbital Interactions in [4+2] cycloadditions, Intramolecular Diels–Alder reactions. Stereochemistry of Electrocyclic Reactions and Sigmatropic rearrangements. Cope rearrangement, Claisen rearrangement and ene-reaction. Pericyclic reactions in Organic synthesis – case studies.

Recommended Books

1. M. B. Smith, Organic Synthesis, 2nd ed., McGraw-Hill, 2000.
2. M. B. Smith, March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure, 7th ed., Wiley, 2013.
3. F. A. Carey, R. J. Sundberg, Advanced Organic Chemistry (parts A and B), 5th ed., Springer, 2008.
4. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
5. N. J. Turro, V. Ramamurthy, J. C. Scaiano, Modern Molecular Photochemistry of Organic Molecules, University Science Books, 2010.
6. E. V. Anslyn, D. A. Dougherty, Modern Physical Organic Chemistry. University Science Books, 2006.
7. H. R. Crabtree, The Organometallic Chemistry of the Transition Metals, 6th ed., John Wiley & Sons, 2014.
8. S. D. Burke, R. L. Danheiser, Handbook of Reagents for Organic Synthesis, John Wiley & Sons, 1999.

24-808-0603 Physical Chemistry III: Electrochemistry and Solid State Chemistry (4 Credits)

L-T-P 4-0-0 Level: 300

Pre-requisite: None

CO	CO Statement	CL
CO1	Describe the theories and mechanism of ionic and electronic conductance and apply the concepts.	Apply
CO2	Explain the basic theory of electroanalytical techniques..	Apply
CO3	Understand basic properties and symmetry of solids	Understand

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	3	2	3	2
CO2	3	3	2	2	2	2
CO3	3	3	2	2	1	1

Module I (10 hrs)

Introduction- Electrochemical Cells, Electrodes, Types of electrodes- Standard hydrogen electrode, Calomel electrode, Quinhydrone electrode. Electrolytes, Half Reactions, Electrochemical Work, Electrodics: Equilibrium electrochemistry- Half- reactions and electrodes, Standard Electrode potential, Nernst Equation. EMF and free energy. Types of cells. Electrochemical series. Liquid junction potential. Ion–Solvent, Ion–Ion Interactions, Ionic and Electronic Conductance, Conductance Measurement, Equivalent Conductance, Kohlrausch's Law, Ostwalds dilution law, Ionic Mobility, Walden's rule, abnormal conductance, Transport Number- Factors Influencing, measurement- Hittorf's and moving boundary methods.

Module II (12 hrs)

Electrode–Ion interface, liquid junction potential, Electrical Double Layer, Electrode and Electrolyte polarization. Overpotential. Butler Volmer Equation. Tafel Plot. Mass transfer control, Charge transfer at electrode-electrolyte interface. Double layer. Electrocapillarity. Hydrogen and Oxygen overvoltage. Activity and Activity co-efficients, Debye-Huckel Theory, Limitations. Extension, Bjerrum ion pair formation. Ionic Atmosphere, Relaxation, Mechanism of Electrolytic Conductance, Debye Huckel Onsager equation for strong electrolytes.

Module III (11 hrs)

The electromotive force, Standard potentials, Applications of standard potentials, Determination of solubility product and activity co-efficient, Activity and Activity Coefficient of Electrolytes.

Corrosion of metals- different forms of corrosion and prevention. Electrochemical Theory of corrosion – methods of prevention. Porbaux and Evans diagram. Fuel Cell, Batteries: Basic theory and types (Elementary idea)

Module IV (12 hrs)

Electroanalytical Techniques: pH determination, Redox indicators principle. Conductometric and potentiometric titrations. Cyclic voltammetry, Square wave, and linear sweep voltammetry, Chronoamperometry, Chronopotentiometry, Impedance. Coulometry and Polarography,

Spectroelectrochemistry (Basic Principles)

Module V (15 hrs)

Crystal structures and symmetry, Crystallographic point groups, space group, unit cells, Miller indices, Seven crystal systems and Bravais lattices, Simple, body centered and face centered systems, Packing in solids- packing diagrams, close packing,- hcp and ccp structures, XRD, Braggs equation – derivation, Powder and rotating crystal technique. Identification of cubic crystals based on interplanar ratio.

Ionic solids with formula MX (CsCl, NaCl, Zinc Blende and Wurtzite Structures), MX2 (Fluorite and Antfluorite Structures, Cadmium Halides, CaF2, Rutile, Anti-rutile, betacristobalite), other crystal systems (Bismuth tri-iodide, Corundum, Rhenium Trioxide etc.), Mixed oxides (Spinel, Perovskite, Ilmenite). The properties of solids**,** Mechanical properties Electrical properties, Impact on nanoscience: Nanowires, Optical properties, Magnetic properties.

Point Defects in crystals- stoichiometric and non-stoichiometric defects, Line defect, surface defects,

Liquid Crystals- Classification and application.

Recommended Books

1. J. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Edn., Wiley, New York, 1998
2. R. Crow, Principles and Applications of Electrochemistry, Paper back edn, 4th edn, 1994.
3. S. Glasstone, An Introduction to Electrochemistry, Paperback Edn., 2007.
4. Skoog, West, Holler, Crouch, Fundamentals of Analytical Chemistry, Wiley, 9th Edn.
5. L.V. Azaroff, Introduction to Solids, Mc Graw Hill, 1960.
6. A. R. West, Solid State Chemistry, Wiley Student (Indian) Ed., (2014)
7. A.K. Galwey, Chemistry of Solids, Chapman and Hall, London, 1967. 35
8. Lesley Smart and Elaine Moore, Solid State Chemistry, Chapman and Hall, 1995
9. H. V. Keer, Principles of the Solid State Wiley Eastern Ltd, New Delhi, 1993.
10. C. N. R. Rao and J. Gopalakrishnan, New Directions in Solid State Chemistry. 2nd Edn, Cambridge Uty Press, 1997.

24-808-0604 Advanced Physical and Inorganic Chemistry Lab (4 Credits)

L-T-P 0-0-8 Level: 300

Pre-requisite: None

CO	CO Statement	CL
CO1	Execute and perform experiments based on pH metry, potentiometry, conductometry and colorimetry.	Evaluate
CO2	Understand the operation principles of various instruments and perform experiments using them	Evaluate
CO3	Apply the concepts of qualitative and quantitative aspects in inorganic preparation	Apply
CO4	Synthesize metal complexes and characterize them by various physicochemical methods.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	3	3	3	3
CO2	3	3	3	3	3	3
CO3	3	3	3	3	3	3
CO4	3	3	3	3	3	3

pH Metry: Acid-base titrations involving strong and weak acids/bases.

Conductometry: Acid-base titrations involving strong and weak acids/base, Determination of degree of ionization of weak electrolytes

Potentiometry: Acid-base titrations involving strong and weak acids/base, Determination of degree of ionization of weak electrolytes. Redox titrations.

Colorimetry: Verification of Beer-Lambert Law, Estimation of ferric iron by colorimetry, Estimation from real samples

Inorganic preparations: Preparation of Tris(oxalato)manganese(III), Tetrapyridinesilver(II) peroxidisulphate, Tris(acetylacetonato) iron(III), Bis(N,N-diethyldithiocarbamato)nitrosyliron(I), Optical isomers of tris(ethylenediamine)cobalt(III)chloride, Nitropentamminecobalt(III) chloride, Tri(acetylacetonato)manganese(III), Tris(thiourea) copper(I) sulphate, Phenyl lithium, Tetraphenyl lead, Ferrocene, Phosphonitrilic chloride

Recommended Textbooks

1. Gurtu, J. N., Gurtu, A., Advanced Physical Chemistry Experiments, 6th Ed.,Pragati Prakashan,2014.
2. Yadav, J. B., Advanced Practical Physical Chemistry, 36th Ed., Krishna Prakashan, 2016.
3. D.P Shoemaker, G.W Garland, J.W Nibler, Experiments in Physical Chemistry, 5th Edn., McGraw Hill.
4. B. P. Levitt, Findlay's Practical Physical Chemistry, 9 th Edn, Longman Group Ltd.
5. Vogel's textbook of quantitative chemical analysis, Fifth Edition
6. A.I. Vogel, A Text Book of Quantitative Inorganic Analysis, Longman, 1966
7. G. Pass, H. Sutcliffe. Practical Inorganic Chemistry 2nd edition, Chapman & Hill. 1974.
8. J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, Vogel's Textbook of Quantitative Chemical Analysis, 6th Edn., Pearson Education, Noida, 2013.

24-808-06YY Visualization and Computing (3 Credits)

L-T-P 1-0-4 Level: 300

Prerequisites: None

CO	CO Statement	CL
CO1	Understand the structures using 3D visualization	Apply
CO2	Build molecule, biomolecules and unit cell	Apply
CO3	Extract structural information from available databases	Analyze
CO4	Calculate and analyse structures and protein ligand binding energies under MM	Analyze

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	1	1	1	0	0
CO2	0	2	1	1	1	1
CO3	0	3	2	2	1	2
CO4	0	3	3	3	3	3

Module I (15 hrs)

Introduction to cheminformatics, Graphical 3D-visualisation of the chemical world using various visualizer tools: Molecules, Biomolecules and Materials. Various file formats, Interconversion of various file formats.

Module II (15 hrs)

Building molecules, biomolecules and materials using softwares. Internal, Cartesian and fractional coordinate systems. Z-matrix, Unit cell and lattice.

Module III (15 hrs)

Introduction to databases – Crystallographic databases, Materials project, PDB database – PDB data, Secondary structure prediction, Fold recognition.

Module IV (15 hrs)

Molecular Mechanics - Force fields - energy calculation, minimization and analysis.

Module V (15 hrs)

Basics of structure based drug design- Docking - Molecular Recognition, Prediction of Protein-ligand interaction sites.

Recommended Text Books:

1. Leach, A.R. “Molecular Modelling Principles and Application, Longman”, 2001.
2. Haile, J.M. “Molecular Dynamics Simulation Elementary Methods,” John Wiley and Sons, 1997.
3. Satya Prakash Gupta, QSAR and Molecular Modeling, Springer - Anamaya Publishers, 2008.
4. Cramer, C. J., “Essentials of Computational Chemistry- Theories and Models”, 2nd Edition, Wiley, 2004
5. Jensen, F., “Introduction to Computational Chemistry”, 3rd Edition, Wiley, 2017.
6. Young, D., “Computational Chemistry – A Practical Guide”, Wiley, 2001.

24-808-0701 Inorganic Chemistry IV: Reaction Mechanism and Organometallic Chemistry (4 Credits)

L-T-P 4-0-0 Level: 400

Prerequisite: 24-808-0501 or equivalent

CO	CO Statement	CL
CO1	Understand the basic concepts and applications of organometallics.	Understand
CO2	Evaluate the structure, bonding and reactions of organometallic compounds and metallocenes.	Analyse
CO3	Predict the stability of organometallic compounds and metal clusters.	Apply
CO4	Explain the stability of transition metal complexes, their reactivity, and the mechanisms of ligand substitution	Analyze
CO5	Explain the application of reactions of organometallic complexes in homogeneous catalytic processes.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	0	0	3	2	2
CO2	3	0	0	3	2	2
CO3	3	0	0	3	2	2
CO4	3	0	0	3	2	2
CO5	3	0	0	3	2	2

Module I (12 hrs)

Organometallic Chemistry. Compounds with transition metal to carbon bonds: eighteen electron rule; classification of ligands, nomenclature, metal-metal multiple bonding, Concept of hapticity of organic ligands. Metal carbonyls: 18 electron rule, EAN rule as applied to carbonyls, electron count of mononuclear, polynuclear and substituted metal carbonyls of 3d series. Preparation and structure of mononuclear and binuclear carbonyls of Cr, Mn, Fe, Co and Ni. π-acceptor behaviour of CO, synergic effect and use of IR data to explain extent of back bonding.

Module II (12 hrs)

σ donor ligands – metal alkyl, aryl complexes; σ donor/π acceptor ligands, – metal alkenyls, alkynyls, carbenes, carbynes, isocyanide, phosphines, fluxionality of ligands – structure, bonding, spectra, preparation and reactions.

σ, π donor/π acceptor ligands – olefin complexes, alkyne, allyl, enyl complexes

Metallocene- ferrocene, titanocene, zircanocene, arene complexes, cycloheptatriene, cyclooctatetraene, cyclobutadiene complexes, fluxionality of ligands – structure, bonding, preparation, reactions and spectroscopy.

Module III (12 hrs)

Metal–Metal bonds and Transition metal clusters; preparation, properties and spectroscopy. Parallels with nonmetal chemistry- isolobal analogy. Application of Wade-Mingos-Lauher rules in predicting the structure of organometallic clusters Organo-lithium aluminium, magnesium, zinc and titanium compounds – their preparations, properties, reactions, bonding and applications.

Spectral analysis and characterization of organometallic complexes.

Module IV (12 hrs)

Reaction Mechanism: Thermodynamic and kinetic consideration, formation constant and rate constant, inert and labile complexes, factors affecting the stability and lability of complexes.

Ligand substitution in octahedral complexes, mechanism of substitution reactions in octahedral complexes, dissociative, associative and interchange mechanism, energy profile of reactions, acid and base hydrolysis, factors affecting the rate of substitution reactions in octahedral complexes.

Ligand substitution in square planar complexes, mechanism of substitution reactions in square planar complexes, energy profile of reactions, the trans effect and its applications, theories for explaining trans effect, factors affecting the rate of substitution reactions in square planar complexes.

Electron Transfer Reactions: inner sphere and outer sphere mechanism, Marcus theory, photochemical reactions

Module V (12 hrs)

Reactions of organometallic complexes – Ligand cone angle, oxidative addition, reductive elimination, insertion, nucleophilic and electrophilic attack of coordinated ligands. Homogeneous catalysis using organometallic compounds: olefin hydrogenation, hydroformylation, Wacker process, Ziegler-Natta polymerisation, cyclo oligomerisation, olefin isomerisation, olefin metathesis, Monsanto acetic acid synthesis, Fischer-Tropsch process, hydrosilylation, coupling reactions in organic chemistry

Recommended Books :

1. Ch. Elschenbroich, A. Salzer, Organometallics – A Concise Introduction, VCH Publishers, 1989.
2. B. D. Gupta, A. J. Elias, "Basic Organometallic Chemistry", University Press, 2010.
3. Powell, Principles of Organometallic Chemistry, 2nd ed., ELBS, 1991.
4. J. E. Huheey, E. A. Keiter, R. L. Keiter, Inorganic Chemistry: Principles of structure and Reactivity, 4th ed., Harper Collin College Publishers, 1993.
5. Basolo, F, and Pearson, R.C., Mechanisms of Inorganic Chemistry, 2nd Ed., John Wiley & Sons, NY, 1967.
6. Crabtree, Robert H. The Organometallic Chemistry of the Transition Metals. 6th Ed., NY: John Wiley, 2014.
7. Miessler, G.L. & Tarr, D. A. Inorganic Chemistry, 5th Ed., Pearson Publication, 2013.
8. D. F. Shriver, P. W. Atkins, C. H. Langford, Inorganic Chemistry, 3rd ed., ELBS, 1999.

24-808-0702 Organic Chemistry IV: Heterocyclic Compounds, Natural Products & Drug Development (4 Credits)

L-T-P 4-0-0 Level: 400

Pre-requisite: None

CO	CO Statement	CL
CO1	Device synthesis scheme for heterocyclic aromatic and nonaromatic organic compounds.	Apply
CO2	Elucidate structure and device synthesis for important natural products.	Apply
CO3	Understand various stages and processes involved in drug discovery and development.	Understand
CO4	Develop natural product-based drug molecules and characterization of complex natural products and biomolecules using spectroscopic techniques	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	2	2	3	2	2
CO2	2	3	2	3	3	2
CO3	2	2	2	3	2	2
CO4	2	2	2	3	2	2

Module I (13 Hrs)

Heterocyclic compounds: Nomenclature of three to seven-membered heterocyclic compounds. Five and six-membered heteroaromatic compounds containing one to four heteroatoms (N, O, S). Indole, quinoline and isoquinoline-structure, general preparation and chemical properties. Flavonoids, coumarin and anthocyanin- structure, properties and biological functions.

Alkaloids: Isolation and classification, isolation, and structure elucidation based on degradative reactions (quinine and atropine). Biosynthesis of quinine and papaverine.

Module II (12 hrs)

Terpenoids: Classification, biosynthesis. Structure and synthesis of abietic acid. Steroids: classification, biosynthesis. Structure and synthesis of cholesterol, conversion of cholesterol to progesterone, androsterone and testosterone. Fatty acids: structure, biosynthesis. Prostaglandins-classification, structure, biosynthesis and synthesis.

Module III (12 hrs)

Carbohydrates: Classification, configurational relationship of monosaccharides—aldotetroses, aldopentoses and aldohexoses. Structure and properties of D-Glucose—Open-Chain Structure, cyclic Structure. Configuration of D-Glucose, Haworth-Projections, conformations of D-glucose. Epimers, mutarotation and its mechanism. Lengthening and shortening of carbon chain of aldoses, Structure of Various Disaccharides—Maltose, Lactose, Cellobiose and Sucrose, Polysaccharides-Starch, Cellulose, Glycogen, Chitin and Heparin.

Preparation of alditols, glycosides (O, C, and N), and deoxysugars. Synthesis of Vitamin C from glucose.

Module IV (13 hrs)

Drug Discovery and Development: Introduction to various phases of drug discovery and development, targets in drug discovery. In-vitro screening systems. Structure-activity relationships, quantitative structure-activity relationships. Pharmacophore, pharmaco-dynamics and pharmaco-kinetics. Dose response parameters-LD50, ED50, LC50, EC50, MIC and MEC. Computer-aided drug design strategies-structure-based drug design, ligand-based drug design. Basics of clinical trials. Mechanism of drug action through examples: Taxol (anticancer agent), penicillin (antibiotic).

Natural product-derived drugs, Synthetic strategies towards plant-based drugs- diversity-oriented synthesis (DOS), biology-oriented synthesis (BIOS) and diverted-total synthesis (DTS).

Module V (10 hrs)

Application of spectroscopic techniques: 2D NMR spectroscopy, chiroptical spectroscopy, characterisation of natural products and biomolecules using spectroscopic techniques including 2D NMR- case study.

Recommended Text Books

1. I. L. Finar, Organic Chemistry Volumes 1 & 2, 6th ed., Pearson Education Asia, 2004.
2. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
3. N. R. Krishnaswamy, Chemistry of Natural Products; A Unified Approach, Universities Press, 1999.
4. S. P. Bhutani, Chemistry of Biomolecules, 2nd ed., CRC Press, 2020.
5. R. O. C. Norman, Principles of Organic Synthesis, 2nd ed., Chapman and Hall, 1978.
6. J. A. Joule, K. Mills, Heterocyclic Chemistry, 5th ed., Wiley, 1998.
7. A. Gürses, M.Açıkyıldız, K. Güneş , M. S. Gürses, Dyes and Pigments, Springer, 2016.
8. K. Stromgaard, P. Krogsgaard-Larsen, U. Madsen, Textbook of Drug Design and Discovery, 5th ed., 2017, Taylor & Francis Group.
9. B. E. Blass, Basic Principles of Drug Discovery and Development, Elsevier, 2015.

24-808-0703 Theoretical Chemistry III: Approximations and Chemical Bonding (4 Credits)

L-T-P 4-0-0 Level: 400
Prerequisite: 24-808-0404 (Quantum Mechanics) or equivalent.

CO	CO Statement	CL
CO1	Derive the Schrodinger equation for multielectronic atoms and interpret the results.	Apply
CO2	Derive the variational principle and perturbation theory, use them to calculate properties for simple systems of chemical interest.	Analyze
CO3	Explain Hartree-Fock Theory and semiempirical Huckel MO treatment and its application to polyelectronic molecules	Analyze
CO4	Classify various basis sets and justify its use for a specific problem	Analyze
CO5	Explain different chemical properties of molecules by drawing molecular orbitals and analyze and interpret the results to solve chemical puzzles.	Analyze

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	1	0	2	1	0
CO2	2	1	0	2	1	0
CO3	3	1	1	3	1	0
CO4	3	2	2	3	2	2
CO5	3	3	3	3	3	3

Module I (14 hrs)

Hamiltonian operators, Wave functions and energy of H like systems, Orbital functions, Postulate of electron spin-orbital and spin functions. Zeeman effect. Spin Orbitals and their construction, Antisymmetric wave functions, Pauli's antisymmetry principle. Many body problems, Born – Oppenheimer Approximations, Independent particle method, Drawbacks. Variational method – theory, proof and general treatment of linear variational problem- Application to systems such as Hydrogen, Helium and various other cases.

Module II (10 hrs)

Hamiltonian operator for multielectronic atom, Perturbation method: Time Independent perturbation for non- degenerate –first order, perturbation corrections to energy and wave functions, Application of this to various systems such as particle in a box, helium atom. Self-Consistent Field approximation- Hartree's proposal, Pauli's antisymm principle, Pauli exclusion principle, Electron spin, Constructing Antisymmetric spin incorporated wave functions for He, excited state of He – various electronic states, term symbols. Hartree-Fock Self Consistent Field method for

multielectronic atoms. The Coulomb and Exchange Operators, The Fock Operator, Koopmans' theorem, Brillouin's theorem, Slater's treatment of complex atoms, Slater orbitals, Slater determinant and wave function.

Module III (8 hrs)

Chemical Bonding- Application to H_2^+, MO and VB treatment of H_2 molecule- Comparison. Concept of σ, σ*, π, π* orbitals and their characteristics, hybrid orbitals, calculation of coefficients of AO used in sp, sp^2 and sp^3 hybrid orbitals, interpretation of geometry, Valence bond model of H_2, Hybridisation of H_2O, BF_3, NH_3 and CH_4 Hartree Fock -Roothaan method - LCAO approximation - Restricted HartreeFock (RHF) for closed shell systems, Restricted open HF (ROHF), and Unrestricted HF (UHF) methods, Empirical, Semi empirical and ab initio methods. Basis functions- Slater Type Orbital and Gaussian Type Orbitals. Contracted and primitive. Basis sets. Minimal, multiple zeta, split-valence, polarized and diffused. Pople style basis sets, designation of basis set size –Dunnings correlation consistent basis sets, Relativistic effects - Effective core potential, ECP.

Module IV (13 hrs)

HMOT: Pi bonding in simple molecules, HMO method for linear conjugated hydrocarbons, linear, cyclic, polycyclic, heterocyclic; ethylene, 1,3-butadiene, allyl radical, cation and anion, aromatic hydrocarbons, cyclopropenyl systems, cyclobutadiene, benzene, naphthalene, thiophene. Calculation of charge distribution, bond orders and reactivity. QMOT: Applications of Molecular Orbital Theory in Understanding reactions and Mechanisms. Qualitative MO theory. Group orbitals. Frontier Orbitals, Substituent effects on frontier orbitals, HSAB concept, Nucleophiles and Electrophiles, Perturbation theory of reactivity. Application of Frontier Orbital theory in studying ionic and radical reactions, Ambident electrophiles, α-effect.

Module V (30 hrs)

Computational calculations listed below using available Molecular orbital theory suite of programme package: Constructing molecular structures or models; Molecular geometry optimization; Conformational analysis; Thermodynamic and spectroscopic properties; Molecular orbital analysis; Electron density and electrostatic potential map.

Recommended Text Books:

1. Atkins, P.W. and Paula, J. Physical Chemistry, 8th Ed., Oxford Press, 2006.
2. Szabo, A.; Ostlund, N. S. "Modern Quantum Chemistry: Introduction to Advanced Structure theory", Dover Publications, 1996.
3. Levine, I. N. "Quantum Chemistry", 7th Edition, Pearson Education Inc., 2014.
4. McQuarrie, D. A., "Quantum Chemistry", 2nd Edition,University Science Books, 2008.
5. Pillar, F. L. "Elementary Quantum Chemistry", 2nd Edition, Dover Publication, 2001.
6. Chandra, A. K., "Introduction to Quantum Mechanics", 4th Ed, Tata McGraw-Hill, New Delhi, 2003.
7. Prasad, R. K., "Quantum Chemistry", 4thEdition, New Age International, 2009.
8. Cramer, C. J., "Essentials of Computational Chemistry- Theories and Models", 2nd Edition,

Wiley, 2004.

9. Jensen, F., “Introduction to Computational Chemistry”, 3rd Edition, Wiley, 2017.
10. Young, D., “Computational Chemistry – A Practical Guide”, Wiley, 2001.
11. Anslyn, E. V.; Dougherty, D. A. Modern Physical Organic Chemistry. University Science Books.
12. Foresman, J. and Frisch, A.,“ Exploring chemistry with electronic structure methods”, Guassian Inc, 2000.

24-808-0704 Scientific Writing and Presentation (2 Credits)

L-T-P 1-0-2 Level: 500

Prerequisite: None

CO	CO Statement	CL
CO1	Apply data analysis tools and logical reasoning in the in-depth study and critical analysis of primary literature data	Apply
CO2	Use basic graphical and sketching tools for data analysis and presentation	Analyze

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	2	2	2	3	3
CO2	1	2	2	2	3	3

Soft Skills: Operating Systems, Document Preparation-Microsoft Word and LaTex. Graph/plotting softwares – Excel, ORIGIN, MATLAB, Veusz; Presentation tools - Powerpoint, , Reference management softwares- Endnote,Mendeley, Refworks
Subject Specific Soft Skills – Building / drawing Molecules - ChemDraw, ChemSketch.

Literature search- Introduction to databases – Scifinder, Reaxys, and Cambridge Structural Databases. Web browsing: various publisher sites such as ACS, RSC, Wiley, Science Direct, Scopus, Web of Science, UGC-INFLIBNET, Shodh Sindu, Shodh Ganga Plagiarism software.

Recommended Books

1. John M. Swales & Christine B. Feak, Academic Writing for Graduate Students, 3rd Edition, Michigan Publishing, 2012.
2. Stephen Bailey, Academic Writing, A Handbook for International Student,5th Edition, Routledge, Taylor & Francis, 2018.
3. Kothari, C. K., Research Methodology-Methods and Techniques, 2nd Ed., New Age International, New Delhi, 2023
4. Montgomery, D. C., Design & Analysis of Experiments, 5th Ed., Wiley India (2007).

24-808-0705 Polymer Chemistry (4 Credits)

L-T-P 4-0-0 Level: 400

Pre-requisite: None

CO	CO Statement	CL
CO1	To gain basic knowledge about various Polymerization mechanism	Understand
CO2	To understand various types of polymerisation techniques and processing.	Understand
CO3	To get knowledge on polymer characterization	Analyze
CO4	To get an idea about the functional polymers and the applications for advanced technologies	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	0	0	3	2	2
CO2	3	0	0	3	2	2
CO3	3	0	0	3	3	2
CO4	3	0	0	3	3	2

Module I (10 hrs)

Introduction. Nomenclature. Classification. Molecular weight. Physical states. Crystalline and amorphous behaviour. Thermal transition. Mechanical properties. Chemical Bonding and Polymer Structure.

Module II (14 hrs)

Polymerization Mechanism. Free radical addition polymerization. Kinetics and mechanism. Chain transfer. Molecular weight distribution and molecular weight control. Cationic and anionic polymerization. Polymerization without termination. Living polymers. Step Growth polymerization. Kinetics and mechanism. Linear Vs cyclic polymerization, Group Transfer, metathesis and ring opening polymerization. Copolymerization. Copolymerization equation, Q-e scheme, Gelation and Crosslinking.

Module III (10 hrs)

Polymerization techniques and Processing. Bulk Solution, melt, suspension, emulsion and dispersion techniques. Elastomers. Fibers. Plastics.

Module IV (14 hrs)

Polymer Characterization. Molecular weights. Concept of average molecular weights, Determination of molecular weights. Gel Permeation Chromatography and Light scattering techniques. Molecular weight distribution. Crystalline and amorphous states. Glassy and Rubbery States. Glass transition and crystalline melting. Degree of Crystallinity, X-Ray diffraction analysis. Thermal analysis of polymers. TG/DTG, DTA/DSC, Spectroscopy of polymers. Microstructure determination by IR, Raman, UV, NMR and MS techniques. Solid State NMR.

Module V (12 hrs)

Functional Polymers. Porous Organic Polymers, Covalent organic framework, Dendritic polymers, Conducting polymers, Redox polymers, Luminescent polymers. Liquid Crystalline polymers.
Industrial polymers. Polyethylene, polystyrene. PVC, PAN, Poly(vinyl carbazole). Silicone polymers.
Polymers for Advanced Technologies. Sensor Applications. Applications in Electronics and Energy – Electrically Conductive Polymers, Polymeric Batteries, Organic Photovoltaic Polymers. Photonic Polymers – Nonlinear Optical polymers, Light Emitting Diodes.

Recommended Books :

1. F. W. Billmeyer Jr., Textbook of Polymer Science, John Wiley and Sons, N.Y. 1991.
2. V. R. Gowarikar, Polymer Chemistry, New Age International Pvt. Ltd., New Delhi, 2010
3. George Odian, Principles of Polymerization, 4th Edn., Wiley, 2004
2. J.M.G Cowie. Polymers, Physics and Chemistry of Modern Materials. Blackie. London, 1992.
3. R.J.Young, Principles of Polymer Science, 3rd ed., Chapman and Hall. N.Y. 1991.
4. R. O. Ebewele, Polymer Science and Technology, CRC Press. N.Y., 1996
5. P.J. Flory, A TextBook of Polymer Science, Cornell University Press, Ithacka, 1953.
6. F. Ullrich, Industrial Polymers, Kluwer, N.Y, 1993.
7. H.G.Elias, Macromolecules, Vol. I & II, Academic, N.Y. 1991.
8. J.A.Brydson, Polymer Chemistry of Plastics and Rubbers, ILIFFE Books Ltd., London, 1966
9. J.R.Fried, Polymer Science and Technology, Pearson Education Inc., New Jersey, 2014.

24-808-0706 SUPRAMOLECULAR CHEMISTRY AND APPLICATIONS (4 Credits)

L-T-P 4-0-0 Level: 400

Pre-requisite: None

CO	CO Statement	CL
CO1	Explain the structural features of any given supramolecular system	Analyze
CO2	Analyze the type of possible interactions in any given host guest assembly	Analyze
CO3	Predict the photochemical and Photophysical behavior in constrained media	Analyze
CO4	Analyze the change in electronic structure of the supramolecular systems based on the interaction with the host	Evaluate
CO5	Utilize the studied systems for applications for catalysis, solar energy conversions, drug delivery etc.	Evaluate

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	3	2	2
CO2	3	2	1	3	2	2
CO3	3	2	1	3	2	1
CO4	3	2	1	3	2	1
CO5	3	2	1	3	2	2

Module I (12 hrs)

Self-assembly and preorganization, Supramolecules non-covalent forces and interactions in supramolecules–Hydrogen bonding, π Effects, dipole interactions, induced dipole interactions, hydrophobic interactions. Solvent Effects, Thermodynamics of binding phenomena.

Module II (12 hrs)

Molecular Recognition – Host guest interactions, Macrocycles, Structure, Preparation and Properties of crown ethers, cryptates, cryptands, carcerands, calixarenes, cyclodextrins, fullerenes, dendrimers, rotaxanes, cucurbiturils.

Module III (12 hrs)

Complex Architectures – Self-assembly, Complementarity and Reorganization, Coordination driven self-assembly of supramolecular two and three dimensional architectures, kinetic and thermodynamic aspects, COF, MOF and their applications.

Module IV (12 hrs)

Photochemistry in constrained media- photophysical, photochemical processes, energy transfer, electron transfer. Effect of structural features and interactions on energy levels.

Module V (12 hrs)

Applications – photocatalysis, water splitting, solar cell, CO_2 reduction, drug delivery, sensors, gas separation and storage.

Recommended Books:

1. Jonathan W. Steed, Jerry L. Atwood, Supramolecular Chemistry, Wiley, 2013.
2. J. M. Lehn, Supramolecular Chemistry: Concepts and Perspectives, Wiley, 1995
3. E.V. Ansyln, D. A. Dougherty, Modern Physical Organic Chemistry, University Press, 2006.
4. P. Klan and J. Wirz, Photochemistry of Organic Compounds,
5. Nicholas J. Turro, V. Ramamurthy, J.C. Scaiano, Modern Molecular Photochemistry of Organic Molecules,
6. Christian S. Diercks, Markus J. Kalmutzki, and Omar M. Yaghi, Introduction to Reticular Chemistry: Metal-Organic Frameworks and Covalent Organic Frameworks, Wiley, 2019.
7. Shengqian Ma, Jason A Perman, Elaboration and Applications of Metal-Organic Frameworks, World Press, 2018.

24-808-0801 Research Proposal Writing (2 Credits)

L-T-P 1-0-2 Level: 500

Prerequisite: 24-808-0704 or equivalent

CO	CO Statement	CL
CO1	Develop skill in writing a scientific proposal/ Review	Create

Research Proposal and Review Writing: Components of a proposal, Work plan, Budget and funding. Types of reports – Communication, full length article and reviews. Publication process, selection of journals, citation index, impact factor, h-index.

Recommended Books

1. John M. Swales & Christine B. Feak, Academic Writing for Graduate Students, 3rd Edition, Michigan Publishing, 2012.
2. Stephen Bailey, Academic Writing, A Handbook for International Student,5th Edition, Routledge, Taylor & Francis, 2018.
3. Kothari, C. K., Research Methodology-Methods and Techniques, 2nd Ed., New Age International, New Delhi, 2023
4. Montgomery, D. C., Design & Analysis of Experiments, 5th Ed., Wiley India (2007).

B. Sc Honors

24-808-0802 Project (4 Credits)

L-T-P 0-0-8

B. Sc Honors with Research

24-808-0802 Project (12 Credits)

L-T-P 0-0-24

Students will undertake the project work according to the regulations of the FYUGP and as approved by the Department Council

24-808-0803 Advanced Analytical and Instrumentation Techniques I (4 Credits)

L-T-P 4-0-0 Level: 500

Prerequisite: None

CO	CO Statement	CL
CO1	Understand the basic principles and instrumentation aspects of various electroanalytical, chromatographic, and thermo-analytical techniques	Understand
CO2	Interpret the data obtained from analytical techniques	Evaluate
CO3	Use the electroanalytical, chromatographic, and thermo-analytical techniques for qualitative and quantitative evaluations	Analyze

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	2	2	2	2
CO2	3	2	2	2	2	1
CO3	3	3	2	2	2	2

Module I (14 hrs)

Potentiometry: different types of indicator electrodes, limitations of glass electrode, applications in pH measurements, other types of ion selective electrodes, solid, liquid, gas sensing and specific types of electrodes, biomembrane, biological and biocatalytic electrodes as biosensors, importance of selectivity coefficients. CHEMFETS- importance of specially designed amplifier systems for ion selective electrode systems. Potentiometric titrations- types and applications.

Module II (14 hrs)

Electrogravimetry- electrogravimetry without potential control, controlled potential electrogravimetry, applications. Coulometry- constant current and constant potential coulometry, applications- primary and secondary coulometry, advantages of coulometric titrations Conductance measurement – conductometric titrations.

Module III (14 hrs)

Polarography – current – voltage curve, DME-components of polarographic current, supporting electrolyte, polarographic maxima. Half-wave potential, Applications of Polarography. Voltammetry - different types, Theory and applications. Stripping analysis. Amperometric titrations – Different types and Applications Impedance spectroscopy, Voltammetric sensors – individual and simultaneous analysis-Case study.

Module IV (12 hrs)

Thermal methods of Analysis TG, DTA and DSC - Instrumentation and Theory – Factors affecting TGA - effect of atmosphere on DTA. TG of copper sulphate pentahydrate and calcium oxalate monohydrate. Application of thermal methods for identification of substances.

Module V (18 hrs)

Solvent extraction and Solid phase extraction, Basic principles of solvent extraction Distribution law- Liquid-liquid extractions, synergistic extraction, Batch extraction, continuous extraction, Counter current extraction, super critical fluids

Chromatography: Basic principles, adsorption, differential migration, effect and choice of stationary and mobile phases, Classification of chromatographic techniques., Thin layer chromatography, Paper chromatography, column chromatography, gas chromatography, ion exchange chromatography, gel permeation chromatography, supercritical fluid chromatography and size exclusion chromatography, Important applications of chromatographic techniques.

Recommended Books:

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
6. C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.
7. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
9. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.
10. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.
11. Contemporary Instrumental Analysis, Kenneth A. Rubinson, Judith F. Rubinson, Prentice Hall, New Jersey, 2000.
12. Wilson & Wilson's, Comprehensive Analytical Chemistry, Volume 47, Modern Instrumental Analysis, Edited by S. Ahuja, N. Jespersen, Reed Elsevier India Private Ltd., Noida, 2006.
13. Journal of Chromatography Library, Volume 3, Liquid Column Chromatography-A Survey of Modern Techniques and Applications, Edited by Z. Deyl, K. Macek, J. Janak, Elsevier Scientific Publishing Company, Amsterdam, 1975.
14. Gas Chromatography, John Willett, John Wiley & Sons, Singapore, 1991.
15. Fundamentals of Analytical Chemistry, Doughlas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Ed., Cengage Learning, 2014.

24-808-0805 Electronic Structure from Molecules to Solids (4 Credits)

L-T-P 4-0-0 Level: 500

Prerequisites: 24-808-0601 or equivalent.

CO	CO Statement	CL
CO1	Construct fragment molecular orbitals, correlation diagrams and interaction diagram.	Analyze
CO2	Explore the effects of symmetry, overlap, and electronegativity in generating the molecular orbital.	Analyze
CO3	Correlate the MO and properties and thus quantify the reactivities	Analyze

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	2	1	2	1	0
CO2	3	2	1	2	1	0
CO3	3	3	2	2	2	2

Module I (14 hrs)

Atomic orbitals, Orbital Interactions leading to molecular orbitals, Molecular orbital coefficients – Degenerate and Non-degenerate Interaction, Electron density distribution. Symmetry consideration, Noncrossing rule. Molecular orbitals of diatomic molecules and electronegativity perturbation.

Module II (12 hrs)

Molecular orbital construction from Fragment orbitals- Linear and circular Hn, Geometrical perturbation and Walsh diagrams. Extending the results to polyenes and cyclic conjugated systems and Huckel's rule of aromaticity.

Module III (12 hrs)

Construction of molecular orbitals of small fragments and their shapes – AH, AH_2, AH_3 and AH_4. Jahn-Teller distortion, Through bond interactions.

Molecules with two heavy atoms- A_2H_6, A_2H_4, and A_2H_2. Polarization and substituent effects.

Module IV (10 hrs)

Transition metal complexes- Octahedral ML_6, square planar ML_4, C_{4v} ML_5 and C_{2v} ML_3 fragments. Isolobal analogy- Generation of isolobal fragments and illustration.

Module V (12 hrs)

Orbitals and Bands, Bloch functions, Reciprocal space and the k quantum number, Band structure – one-dimensional systems, Band width, Fermi level, Higher dimensions, Density of States (DoS)- Basic electron partitioning, Pierl's distortion, Folding Bands, Crystal Orbital Overlap Population (COOP), Constructing and analysing the band structure- Case study –Bulk solid and surface (Adsorption).

Recommended Text Books:

1. T. A. Albright, J. K. Burdett, M.-H. Whangbo, Orbital Interactions in Chemistry, 2nd ed., John Wiley and Sons, Inc., Hoboken, New Jersey, 2013.
2. I. Flemming, Molecular Orbitals and Organic Chemical Reactions, Students ed., Wiley, 2009.
3. A. Rauk, Orbital Interaction Theory of Organic Chemistry, 2nd ed., WileyBlackwell, 2000.
4. W. L. Jorgensen, L. Salem, The Organic Chemist's Book of Orbitals, Academic Press, 1973.

24-808-0806 Advanced Organic Chemistry I (4 Credits)

L-T-P 4-0-0 Level: 500
Prerequisites: 24-808-0602 or equivalent

CO	CO Statement	CL
CO1	Analyze the conformational effects on the reactivity of reactions.	Apply
CO2	Analyze the reagents and conditions for the synthesis of specific target molecules.	Analyse
CO3	Describe strategies for the stereospecific /stereoselective organic transformations towards chiral target molecules.	Apply
CO4	Construct a synthetic pathway for simple to complex organic molecules by retrosynthetic approach.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	1	3	2	1	1
CO2	2	1	3	2	1	1
CO3	1	3	3	2	1	1
CO4	1	3	3	2	1	1

Module I (14 hrs)
Reaction mechanisms and conformational effects on reactivity - Ester hydrolysis, alcohol oxidations, S_N2 reactions, elimination reactions, epoxidation by intramolecular closure of halohydrins, strain-modulated reactivity, epoxide openings (S_N2), electrophilic additions to olefins, rearrangement reactions, conformational and stereoelectronic effects on reactivity.
Stereoselective reactions of cyclic compounds. Reactions on small rings. Stereochemical control in six-membered rings. Stereochemistry of bicyclic compounds. Reactions with cyclic intermediates/transition states.

Module II (12 hrs)
Asymmetric Synthesis: Introduction to asymmetric synthesis, principle, general strategies, chiral pool strategy, chiral auxiliaries, chiral reagents – Binol derivatives of $LiAlH_4$, chiral catalysts – CBS catalyst. Stereospecific and stereoselective synthesis, determination of enantiomeric and diastereomeric excess. Stereoselective nucleophilic additions to acyclic carbonyl groups- Cram's Rule, Felkin-Ahn Model, Effect of chelation on selectivity. Application of asymmetric synthesis in the industrially relevant molecules such as L-DOPA, (S)-metolachlor and menthol.

Module III (10 hrs)
Protecting groups- protection and deprotection of hydroxyl, carboxylic acids, and carbonyls in aldehydes and ketones, amines, alkenes and alkynes. Chemo- & regioselective protection and deprotection. Functional group equivalents, reversal of reactivity (Umpolung).

Module IV (14 hrs)

Disconnection approach-introduction to retrosynthesis, basic principles, synthons, and synthetic equivalents. Monofunctional and bifunctional disconnection, One group C-X and two groups C-X disconnections, one group C-C and two groups C-C disconnections. Computers in organic synthesis – introduction to softwares –SYNTHIA, MAPOS, AiZynthFinder.

Module V (10 hrs)

Retrosynthetic analysis: Longifoline, Corey lactone, Djerassi - Prelog lactone and D-luciferin. Application of AiZynthFinder to retrosynthetic analysis.

Recommended Text Books

1. P. S. Kalsi: Stereochemistry, Conformation and Mechanism, 3rd Edn., New Age Publications.
2. E. L. Eliel and S. H. Wilen: Stereochemistry in Organic Compounds, 1994, John Wiley.
3. J. Clayden, N. Green, S. Warren, P. Wothers, Organic Chemistry, 2nd ed., Oxford University Press, 2012.
4. P. S. Kalsi, Stereochemistry, Conformation and Mechanism, 9th ed., New Age Publications, 2017.
5. S. Warren, Organic Synthesis: The Disconnection Approach, 2nd ed., John Wiley, 2008.
6. E. Robert, Gawley, J. Aube, Principles of Asymmetric Synthesis, 2nd ed., Elsevier, 2012.
7. T.W. Greene, P. G. M. Wuts, Protecting Groups in Organic Synthesis, 2nd ed., John Wiley, 1991

24-808-0807 Materials Chemistry (4 Credits)

L-T-P 4-0-0 Level: 400
Prerequisites: None

CO	CO Statement	CL
CO1	To acquire basic knowledge on various types of materials	Understand
CO2	To gain insight on the structure – property relationship of different materials.	Understand
CO3	To get knowledge on various characterization techniques.	Analyze
CO4	To get an idea about the materials in advanced technological applications	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	0	0	3	2	2
CO2	3	0	0	3	2	2
CO3	3	0	0	3	3	2
CO4	3	0	0	3	3	2

Module I (12 hrs)
Chemistry of Materials. Ionic and covalent solids. Molecular and metallic solids. Amorphous and crystalline materials. Crystalline state. Structural organization of crystalline solids-theories of bonding. Crystal structures. Imperfections in crystal structures.
Semiconductor materials- properties and types of semiconductors. Structure and Bonding of semiconductor materials. Silicon based semiconductors. II-VI (wide band gap) and III-V (narrow band gap) compound semiconductors. Electrical, optical and magnetic properties of semiconductor materials. Preparation and properties of ZnO, ZnS, CdS, CdTe, Ga-As, In-S, Cu-In-S. Application in photovoltaic devices.

Module II (10 hrs)
Polymer Materials- classification and nomenclature of polymers. Methods of Polymerization. Structure–property relationships. Plastics and elastomers. Viscoelastic behaviour. Rubber like elasticity. Crystalline and amorphous polymers. Glass transition temperature and crystalline melting. Functional Polymers.

Module III (12 hrs)
Nanomaterials. Materials in the nanodomain. Zero, one- and two-dimensional materials. Particle size dependent change in properties of materials. Metals in the nanodomain. Gold and silver nanoparticles. Preparation, properties and applications. Core shell structures. Semiconductor nanoparticles. Quantum dots. ZnO, ZnS, CdS and CdSe quantum dots.
Electrical and optical properties. Nano domains of Carbon-fullerenes, carbon nanostructures, graphene, graphene quantum dots.

Module IV (14 hrs)
Characterization of Materials. Optical Microscopy- Principles, instrumentation and application of confocal Raman microscopy, SPM/STM. Electron microscopy- SEM, FESEM, TEM. Principles,

instrumentation and applications. Surface and core level techniques- Photoelectron spectroscopy - X-Ray and UV. Thermal methods- TG/DTG, DTA, DSC, DMA. X-Ray Diffraction

Module V (12 hrs)

Materials in Advanced Technology. Organic Polymer Semiconductors, Solid ionic conductors - Advanced materials for energy generation and energy storage. Porous membranes. Optical and photonic materials.

Recommended Books:

1. B. D. Fahlman, Materials Chemistry, 2nd ed. Springer, Heidelberg, 2011.
2. Harry R. Allcock, Introduction to Material Chemistry, John Wiley & Sons, Inc., New Jersy, 2008
3. R. Zallen, Physics of Amorphous Solids, Wiley, New York, 1983.
4. R. J. Borg, G. J. Dienes, The Physical Chemistry of Solids, Academic Press, Boston, 1993.
5. D. Kingery, H. K. Bowen, D. R. Uhlmann, Introduction to Ceramics, 2nd ed., Wiley, New York, 1992.
6. J. M. J. Cowie, Polymers. Physics and Chemistry of Modern Materials, 3rd ed., CRC Press, Boca Raton, 2007.
7. S. O. Kasap, Principles of Electronic Materials and Devices, Mc Graw Hill, 2006

24-808-0808 Transition Metals: Chemistry and Applications in Organic Synthesis (4 Credits)

L-T-P 4-0-0 Level: 400

Prerequisites: 24-808-0602 or equivalent

CO	CO Statement	CL
CO1	Describe the structure, bonding and properties of transition metal complexes.	Understand
CO2	Predict and explain the principle and mechanism involved in transition metal-mediated transformations.	Apply
CO3	Construct organic molecules for various applications using palladium reagents.	Apply
CO4	Predict the structure and reactions of various metal-carbene complexes.	Apply
CO5	Apply transition metal complexes for various asymmetric transformations	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	1	2	2	1	1
CO2	3	1	2	3	1	2
CO3	1	1	3	3	1	2
CO4	3	1	3	3	1	2
CO5	1	1	3	3	1	2

Module I (12 hrs)

Basic concepts in organometallic chemistry: Introduction, 18 electron rule and its limitations, electron counting with examples, oxidation state, types of ligands, bonding, back-bonding. Formation of transition metal complexes, coordination number and geometry. s-Bonded and p-bonded organometallic compounds.

Module II (12 hrs)

Mechanisms involved in transition metal chemistry: Oxidative addition, reductive elimination, transmetallation, migrative insertion, β-hydride elimination, nucleophilic and electrophilic attack on transition metal complexes. C-H activation. Catalytic mechanism of hydrogenation and hydroformylation. Single electron transfer and radical reactions. Homogeneous and heterogeneous catalysis.

Module III (14 hrs)

Reactions mediated by palladium-based reagents: Characteristics of organopalladium compounds, catalysts and precursors, mechanistic features of cross-coupling reactions, reactivity of substrates, selectivity. Palladium catalysed coupling reactions: Corriu-Kumada reaction, Hiyama reaction, Suzuki coupling, Sonogashira coupling, Heck reaction, Buchwald–Hartwig coupling, Negishi coupling, Stille

coupling. Miscellaneous reactions catalysed by palladium- Direct arylation, cyanation, carbonylation, Tsuji-Trost allylic substitution, α-allylic alkylation and α-fluorination.

Module IV (12 hrs)

Transition metal carbene complexes: Structure and properties. Fischer carbene complexes-preparation and reactions. Schrock carbene complexes-preparation and reactions. Non-stabilised carbene complexes. Metathesis process of carbene complexes

Module V (10 hrs)

Transition metals in asymmetric catalysis: Asymmetric catalysis in metathesis, epoxidation, allylation, hydroformylation, isomerisation of allylic amines, hydrocyanation, hydrogenation, Heck reaction and Pauson–Khand reaction.

Recommended Text Books

1. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, 6th Edn., John Wiley & Sons, 2014.
2. L. S. Hegedus, B. C. G. Soderberg, Transition Metal in the Synthesis of Complex Organic Molecules, 3rd Edn., University of Science Books, 2010.
3. D. Astruc, Organometallic Chemistry and Catalysis, Springer, 2007.
4. J. Tsuji, Transition Metal Reagents and Catalysts: Innovations in Organic Synthesis, John Wiley & Sons, 2002.
5. I. Omae, Applications of Organometallic Compounds, John Wiley & Sons, 1998
6. R. Bates, Organic Synthesis Using Transition Metals, 2nd Edn., John Wiley & Sons, 2012.
7. B. Gabriele, Organic Synthesis *via* Transition Metal-Catalysis, MDPI, 2022.
8. K. Grela, Olefin Metathesis, John Wiley & Sons, 2014.

24-808-0901 Advanced Analytical and Instrumentation Techniques II (4 Credits)

L-T-P 4-0-0 Level: 600

Prerequisites: None

CO	CO Statement	CL
CO1	Gain an in-depth understanding of working principles of advanced analytical and surface characterization techniques.	Understand
CO2	Choose and optimize the right techniques and instrumentation configuration for a particular analysis	Evaluate
CO3	Analyse the data for differentiation and quantitative evaluation of analytes and surfaces	Analyse
CO4	Predict the structure and reactions of various metal-carbene complexes.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	3	2	2	2	2
CO2	2	3	2	1	2	1
CO3	3	2	2	3	2	2

Module I (14 hrs)

Gas chromatography – basic instrumental set up-inlets, carriers, columns, detectors and comparative study of TCD, FID, ECD, NPD and MS. Qualitative and quantitative studies using GC, Preparation of GC columns, packet columns and capillary columns, selection of stationary phases of GLC, Choosing the parameters-Temperature, Length of the column, Sample size, Flow rate, CHN analysis
by GC, Case study.

Module II (14 hrs)

Capillary electrophoresis-migration rates and plate heights, instrumentation, sample introduction, detection methods, applications. Capillary gel electrophoresis. Capillary isotachophoresis. Isoelectric focusing.
Capillary electro chromatography-packed columns. Micellar electro kinetic Chromatography.

Module III (16 hrs)

Separation process, Eddy diffusion, Mass transfer, Longitudinal diffusion, Retention parameters in HPLC-Capacity factor, Retention time, Retention volume, Peak width, Total number of theoretical plates, Height equivalent of a theoretical plate, Resolution and retention time, Solvent delivery systems, Detectors
Instrumentation and functioning of HPLC, Types of HPLC - Modes of separation in HPLC- adsorption chromatography, reversed phase chromatography, ion pair chromatography, ion exchange
chromatography Solubility and retention in HPLC. Method development in HPLC - Selection of mobile phase and optimization, Preparation of sample, Selection of column and solvent, HPLC method validation, HPLC Analysis -Case study Dos and
Don'ts in HPLC - Troubleshooting in HPLC

Module IV (14 hrs)

Measurement of alpha, beta, and gamma radiations, neutron activation analysis and its applications. Principle and applications of isotope dilution methods, Radioimmunoassay (RIA), Immunoradiometric assay (IRMA), Enzyme linked immunosorbent assay (ELISA)-Principles and practical aspects

Module V (14 hrs)

Chemical Analysis of surfaces: Surface preparations-ion scattering spectrometry secondary ion scattering microscopy (SIMS)-Auger election spectroscopy-ESCA instrumentation and application. Electron Microscopies, Basic principles of TEM and SEM, Elemental analysis, XRD, Scanning probe microscopies an overview, Basic principles of AFM and STM, Case study.

Recommended References:

1. J.M. Mermet, M. Otto, R. Kellner, Analytical Chemistry, Wiley-VCH, 2004.
2. D.A. Skoog, D.M. West, F.J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edn., Saunders College Pub., 2007.
3. J.G. Dick, Analytical Chemistry, R.E. Krieger Pub., 1978.
4. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Pub., 1990.
5. G.H. Jeffery, J. Bassett, J. Mendham, R.C. Denney, Vogel's Text Book of Quantitative Chemical Analysis, 5th Edn., John Wiley& sons,1989.
6. C.L. Wilson, D.W. Wilson, Comprehensive Analytical Chemistry, Elsevier, 1982.
7. G.D. Christian, J.E. O'Reilly, Instrumental Analysis, Allyn & Bacon, 1986.
8. R.A. Day, A.L. Underwood, Quantitative Analysis, Prentice Hall, 1967.
9. H.A. Laitinen, W.E. Harris, Chemical Analysis, McGraw Hill, 1975.
10. F.W. Fifield, D. Kealey, Principles and Practice of Analytical Chemistry, Blackwell Science, 2000.
11. Contemporary Instrumental Analysis, Kenneth A. Rubinson, Judith F. Rubinson, Prentice Hall, New Jersey, 2000.
12. Wilson & Wilson's, Comprehensive Analytical Chemistry, Volume 47, Modern Instrumental Analysis, Edited by S. Ahuja, N. Jespersen, Reed Elsevier India Private Ltd., Noida, 2006.
13. Journal of Chromatography Library, Volume 3, Liquid Column Chromatography-A Survey of Modern Techniques and Applications, Edited by Z. Deyl, K. Macek, J. Janak, Elsevier Scientific Publishing Company, Amsterdam, 1975.
14. Gas Chromatography, John Willett, John Wiley & Sons, Singapore, 1991.
15. Fundamentals of Analytical Chemistry, Doughlas A. Skoog, Donald M. West, F. James Holler, Stanley R. Crouch, 9th Ed., Cengage Learning, 2014.

24-808-0902 Advanced Instrumentation Lab (4 Credits)

L-T-P 0-0-8 Level: 600

Prerequisites: None

CO	CO Statement	CL
CO1	Understand the operation principles of various instruments and perform experiments using them	Evaluate
CO2	Quantitative estimation of chemicals using various instruments	Apply
CO3	Estimate essential material properties	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	2	3	3	3	2	2
CO2	2	3	3	3	2	2
CO3	2	3	3	2	2	2

Module 1: (30 hours)
Colourimetry, UV-VIS spectroscopy and Diffuse reflectance spectroscopy: hands on training on the instrument, preparation of stock solutions, verification of Beeer-Lambertz law, Estimation of unknown concentration, establish correlation between molecular structure and spectrum, Band Gap Estimation of thin films, smartphone spectroscopy and comparison with colorimetry and UV-VIS spectroscopy
Fluorescence spectroscopy: Emission Excitation spectral analysis, Fluorescence quantum yield, fluorescence lifetime, quenching

Module II: (20 hours)
Refractometry and Polarimetry: hands on training on the instrument, preparation of stock solutions, estimation of refractive index and optical activity, estimation of unknown concentration, analysis of food samples

Module III (30 hours)
vibrational spectroscopy: hands on training on the instrument, preparation of samples, IR and Raman spectroscopic characterization of organic and inorganic samples, assignment of peaks to functional groups, spectral processing, data processing, chemometry and machine learning tools., preparation of nanomaterials of surface enhanced Raman spectroscopy, comparative study of Raman and SERS

Module IV: (20 hours)
Cyclic voltammetry: determination oxidation-reduction potentials, HOMO and LUMO levels
TGA-DTA Thermal analysis of samples
Gas chromatography and high performance liquid chromatography: sample preparation, separation, qualitative and quantitative analysis

Module V (20 hours)
Estimation of water quality parameters: pH, conductivity, Total Dissolved Solids, hardness, turbidity, Dissolved oxygen, COD, chloride

1. J. N. Gurtu, and A. Gurtu Advanced Physical Chemistry Experiments, 6 th Edn., Pragati Prakashan, 2014.
2. Krishna Chattopadhyay and Manas Mandal ANALYTICAL CHEMISTRY SKILL ENHANCEMENT COURSE, CBSCBS Publishers & Distributors, 2022
3. B. P. Levitt, Findlay's Practical Physical Chemistry, 9 th Edn, Longman Group Ltd.
4. Vogel's text book of quantitative chemical analysis, Fifth Edition.

24-808-0904 Computational Material Chemistry (4 Credits)

L-T-P 4-0-0 Level: 500

Prerequisites: 24-808-0703 (Approximations and Chemical Bonding) or equivalent

CO	CO Statement	CL
CO1	Appreciate the basics of for quantum chemical calculations for materials	Apply
CO2	Distinguish and apply various methods and basis sets for materials	Apply
CO3	Understand and interpret the band structure of any dimensional materials	Analyse
CO4	Practice and interpret the computed results of various sample materials	Analyse

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	3	1	0	2	1	0
CO2	3	2	2	2	2	2
CO3	3	2	2	2	2	2
CO4	3	3	3	3	3	3

Module I (10 hrs)

Basics: Schrodinger's Equation – Periodic Potentials - Bloch Functions – Bonding in Hn systems Reciprocal Space and k Quantum number – Brillouin Zone

Module II (10 hrs)

Band Structures: One-dimensional systems (H_n, N_n, $(H_2)_n$, $[Pt(CN)_4]^{2-}$ systems), Properties of Bands – Band width, Fermi level Interpreting the properties; Structural Distortions; Higher Dimensions; Density of States.

Module III (12 hrs)

Bonds: Basic Electron Partitioning, Energy-resolved Electron and Energy Partitioning, COOP curves and how to interpret these. Electron localization, correlation and exchange energies

Module IV (14 hrs)

Methods and Basis sets: Exchange correlation density functionals. Local density approximation (LDA), density Gradient corrections (GGA). Hybrid and meta–GGA functionals. All electron basis, atomic basis, plane wave basis, Pseudopotential; Normconserving, ultrasoft, PAW

Module V (14 hrs)

Applications Solid state sample problems- Calculating various properties - Structure and energetics, Structural alternative and physical properties; Interpreting the results of material calculations

Recommended Text Books:

1. Hoffmann, R. *Solids and Surfaces*, Wiley-VCH, NY, 1988
2. Cramer, C. J. Essentials of Computational Chemistry, John-Wiley & Sons, 2004.
3. Dronskowski, R. Computational Chemistry of Solid State Materials, Wiley-VCH, 2005
4. Cramer, C. J., "Essentials of Computational Chemistry- Theories and Models", 2nd Edition, Wiley, 2004.
5. Foresman, J. and Frisch, A.," Exploring chemistry with electronic structure methods", GuassianInc, 2000.
6. Jensen, F., "Introduction to Computational Chemistry", 3rdEdition, Wiley, 2017.
7. Leach, A. R., "Molecular Modeling – Principles and Applications", Addison Wesley Longman, 2001
8. Young, D., "Computational Chemistry – A Practical Guide", Wiley, 2001

24-808-0905 Advanced Organic Chemistry II (4 Credits)

L-T-P 4-0-0 Level: 500

Prerequisites: 24-808-0806 or equivalent

CO	CO Statement	CL
CO1	Apply organocatalysts for various organic synthesis	Apply
CO2	Design and synthesis suitable heterogeneous catalysts for various synthetic applications.	Apply
CO3	Understand biorthogonal chemistry and its applications	Understand
CO4	Design and construct suitable polymers with the required properties for different applications.	Apply
CO5	To design and synthesise functional organic materials for specific applications.	Apply

CO No	PSO1	PSO2	PSO3	PSO4	PSO5	PSO6
CO1	1	1	2	3	1	2
CO2	1	1	2	3	1	2
CO3	1	1	2	2	1	2
CO4	1	1	2	2	2	2
CO5	1	1	2	2	2	2

Module I(10 hrs)

Organocatalysis: Introduction to organo-catalyzed reactions, amine, iminium, enamine and carbene-based catalysis reactions. Organocatalysis for asymmetric synthesis.

Module II (12 hrs)

Heterogeneous catalysis: introduction, immobilization and solid supports, metal catalysts (single atoms and nanoclusters), organometallic compounds, magnetically active heterogeneous catalysts**.**

Module III (12 hrs)

Introduction to bioorthogonal chemistry: concept, various ligation strategies *viz.*, 1,3-dipolar cycloaddition of azides with cyclooctynes and nitrones with cyclooctynes; oxime/hydrazone formation from aldehydes and ketones, the tetrazine ligation, the isocyanide-based click reaction, and the quadricyclane ligation.

Module IV (13 hrs)

Polymers for advanced technologies: Liquid-crystalline and high-performance polymers, functional polymers, Polymers for drug release and drug carrier systems, Polymeric gels and networks.

Synthesis and applications of conducting polymers: PPVs, polyaniline (PANI) and polythiophene, polycarbazole, polyacetylene-synthesis and applications (sensor and LED). Polymers in solar cell application

Module V (13 hrs)

Functional organic materials: Organic materials for photovoltaic application. Organic electronic luminescent materials. Synthesis of porphyrins and their opto-electrochemical properties.

Introduction to nonlinear optics, molecules for NLO and imaging. Organic molecular switches.

Design, synthesis and functions of Metal-Organic Framework (MOF) and Covalent Organic Framework (COF).

Recommended Text Books

1. L. Albrecht, A. Albrecht, L. Dell'Amico, Asymmetric Organocatalysis: New Strategies, Catalysts, and Opportunities, Wiley-VCH, 2022.
2. MacMillan, D. The Advent and Development of Organocatalysis, Nature, 2008, 455, 304–308.
3. W. Y. Teoh, A. Urakawa, Y. H. Ng, P. Sit, Heterogeneous Catalysts: Advanced Design, Characterization and Applications, WILEY-VCH GmbH, 2021.
4. F. Zaera, Molecular Approaches to Heterogeneous Catalysis, 2021, 214179.
5. Scinto, S. L., Bilodeau, D. A., Hincapie, R. *et al*. Bioorthogonal Chemistry. Nat. Rev. Methods Primers 1, 30 2021.
6. R. E. Bird, S. A. Lemmel, X. Yu, Q. A. Zhou, Bioconjugate Chemistry, 2021, 32, 2457-2479.
7. J. R. Reynolds, B. C. Thompson, T. A. Skotheim, Conjugated Polymers, Perspective, Theory, and New Materials, 4th ed., 2019, Taylor & Francis Group.
8. W. Hou, Y. Xiao, G. Han, J.-Y. Lin, The Applications of Polymers in Solar Cells: A Review. Polymers 2019, 11, 143.
9. V. F. Yusuf, N. I. Malek, S. K. Kailasa, Review on Metal–Organic Framework Classification, Synthetic Approaches, and Influencing Factors: Applications in Energy, Drug Delivery, and Wastewater Treatment, ACS Omega, 2022, 7, 44507-44531.
10. T. J. J. Müller and Uwe H. F. Bunz, Functional Organic Materials- Syntheses, Strategies and Applications, WILEY-VCH, 2007.
11. M. S. Lohse, T. Bein, Covalent Organic Frameworks: Structures, Synthesis, and Applications, Advanced Functional Materials, 2018, 22, 1705553.
12. Introduction to Organic Electronic and Optoelectronic Materials and Devices by Sam-Shajing Sun, Larry R. Dalton, CRC Press, 2008.
13. Organic Optoelectronics by Wenping Hu, John Wiley and Sons, 2013.
14. Organic Electronics Materials and Devices by S. Ogawa, Springer, 2015.
15. A Journey Through the World of Molecular Machines by C. Davis, Create Space, 2010.
16. Molecular Machines and Motors: Recent Advances and Perspectives by A. Credi, S. Silvi and M. Venturi, Topics in Current Chemistry (Springer), 354, 2014.

24-808-1001 Major Project (20 Credits)

The students shall carry out research project in the Department/reputed research laboratory for the entire semester. The students shall submit a project report on the research work carried out.

The students will have to present the results of the research project in a seminar and appear for a comprehensive viva-voce. A course viva will also be conducted along with project evaluation.

24-808-1002 MOOC Course (4 Credits)

Department council will approve a list of MOOC courses to be taken by students. The students can take a course 4 credits or two courses of two credits. The students can take the course during previous semester and credits can be added to the grades of tenth semester.