Veer Bahadur Singh Purvanchal University
Jaunpur

Syllabus for

Master of Science (M.Sc.) Programme

in Chemistry

Designed as per Syllabus Development Guidelines

Under

National Education Policy 2020

***w.e.f.* 2022-23 (for Campus)**

23.9.22 23/09/2022 23/09/2022 23-9-22

Department of Chemistry

Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research,
V.B.S. Purvanchal University, Jaunpur-222003 UP, India

Ordinance governing two-year (four semesters) postgraduate degree (M.Sc.)

The following ordinances have been framed governing the admission, course structure, examination and other allied matters relating to the two-year (four semesters) postgraduate degree programme (M.Sc.) in Chemistry being offered by **Prof. Rajendra Singh (Rajju Bhaiya) Institute of Physical Sciences for Study and Research,** V.B.S. Purvanchal University. The University adopted the semester and credits-based courses w.e.f. session 2022-23.

A. ADMISSION

1. All matters relating to admission to this course shall be dealt with by the Admission Committee constituted for the purpose by the University.
2. A candidate, who has passed B.Sc. with Chemistry as a subject up to third year from a recognized university is eligible for admission.
3. The intake of students in these programmes shall be fixed by V.B.S. Purvanchal University. The reservation norms for admission shall be guided by State Government notification issued from time to time.
4. On selection the candidates shall deposit the fees prescribed for the purpose to get his/her admission confirmed within the time period fixed by the Admission Committee of the Department. If a candidate fails to do so his/her admission shall be automatically cancelled and the seat falling vacant shall be offered to other candidates as per the merit/category. However, matter concerning fees of candidates under SC/ST category would be governed by Govt. Order; as such there is no provision of fee concession/exemption/refund.
5. Admission to M.Sc. course cannot be claimed by any candidate as a matter of right. The Admission Committee shall have power to refuse, reject or cancel any admission if it possesses sufficient reasons to do so.

B. COURSES OF STUDY AND EXAMINATION

6. To conduct the M.Sc. (Chemistry) programme systematically and within a time bound frame, the concerned Department shall draw up an "Academic Calendar" in the beginning of academic session and shall get it approved by the Vice-Chancellor of the University for its Strict Implementation.
7. A candidate admitted to the M.Sc. course shall pursue a regular course of study in all the four semesters of the course and attend at least 75% of the classes held to be eligible to appear in the examination.
8. If a student fails to attend requisite classes in a semester due to illness, he/she may be given relaxation of 15% attendance (10% at the level of Vice-Chancellor and 5% at the level of Head of Department on production of medical certificate).
9. The examination for semester system in M.Sc. Course in Chemistry shall be by means of theory papers and practical as specified in the examination scheme which consist of:
   (a) Four theory papers and one practical examinations in each of the Seventh, Eighth, Ninth and tenth semesters.
   (b) It is also necessary to do a project work in each semester under the guidance of a faculty member of the department.
10. All papers (Theory and Practical) will be of 4 credits (25% Internal + 75% External) except stated otherwise. Project will be of 4 credits and maximum 100 marks. Duration for examination of a paper will be of 3 hours.

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11. Students are required to take a minor elective (other than own department/faculty) and pass it in seventh or eighth semester (first year of M.Sc.) for the completion of M.Sc. Chemistry Programme.

12. The Departmental Committee/Department shall assign a topic for Project Work/ dissertation/survey along with a supervisor to a candidate in the beginning of second semester which will continue up to fourth semester.

13. An evaluation of project work will be carried by a board of examiners consisting of an external examiner and an internal examiner (supervisor). The Board of Examiners will consist of one External and one/two internal examiners(supervisor) recommended for appointment by the BoS/HoD of department.

14. The name of the candidates successful in the semester system in M.Sc. Course in Chemistry examination shall be arranged in the following grade system:

लैटर ग्रेड	विवरण	अंको की सीमा	ग्रेड पॉइंट
O	Outstanding	91-100	10
A^+	Excellent	81-90	9
A	Very good	71-80	8
B^+	Good	61-70	7
B	Above Average	51-60	6
C	Average	41-50	5
P	Pass	36-40	4
F	Fail	0-35	0
AB	Absent	Absent	0
Q	Qualified		
NQ	Not Qualified		

15. Matters pertaining to the syllabi and conduct of examination shall be dealt with by the Board of Studies (BOS) constituted by the Vice-Chancellor.

16. The BOS shall recommend the panel of paper setters/examiners to the Vice-Chancellor. After getting approval from the Vice-Chancellor, the appointment letters shall be issued to the concerned paper setters/examiners by the Registrar/Controller of Examination of Purvanchal University.

17. Papers for theory examination in sealed covers shall be handed over/sent by registered post to the Registrar/Controller of Examination by the Examiners. Controller of Examinations/Technical Cell will ensure the printing of papers and fair conduct of the examinations.

18. The question papers shall be moderated by a committee consisting of the head and two senior most teachers of the department and the teacher of concerned paper.

19. After the examinations, Controller of Examinations/Technical Cell for campus courses shall ensure the evaluation of the answer books and declaration of results of semester examinations within a reasonable time so as to enable the department to adhere to the Academic Calendar.

20. Practical examinations of semester VII, VIII, IX and X shall be conducted by at least one internal and one external examiner carrying 100 marks in each semester.

21. The students of M.Sc. course shall be examined in the subjects in accordance with course curriculum given at the end of ordinance.

C. RESULTS, PROMOTION AND IMPROVEMENT

22. The pass marks in each semester shall be (i) 36% marks in each theory papers subject to 36% marks in the total of theory. (ii) 36% marks in practical examinations (iii) 40% marks in project works.

23. If a student fails in more than 5 papers in an academic year, he/she will not be promoted to next year. Such student should be re-admitted as Ex. Student with coming batch and their seat will be additional.

24. Students, who failed in 5 or lower number of papers in the academic year will be awarded 'back' and given chances to reappear and pass in respective paper(s) in next 3 years with regular semester examination.

Programme Title: Master of Science (M.Sc.) in Chemistry

Duration and Credit: 2 years (4 Semesters) regular programme with total 100 credits.

Programme Objectives: Programmes objectives are as:

1. To facilitate the students to learn about the various type reactions, periodic properties of elements, bioinorganic, coordination chemistry and structure of molecules, physical properties of compounds, natural products by using theories and instruments
2. To make the students to learn about the physical aspects of atomic structure, dual behaviour, reaction pathways with respect to time, various energy transformations, molecular assembly at nano level, significance of electrochemistry, molecular segregation using their symmetry
3. To learn about the potential uses of organic, inorganic, analytical, polymer and medicinal chemistry in different areas
4. To understand and apply the principles of organic chemistry for understanding the physiochemical relationship and reaction mechanisms, stereochemistry, asymmetric organic synthesis, instrumental method of chemical analysis and separation techniques
5. To help the students for developing the ability to see the structure in 3 D model of molecules via computational chemistry software.
6. To encourage interest in research and development (R&D) and provide to exposure to various research area.
7. To trained the student in various qualitative and quantitative analysis of organic and inorganic compounds
8. To get enormous job opportunities at all level of chemicals, pharmaceutical, food products and polymer industries

Programme Outcomes: Programme outcomes are as:

PO-1. In terms of knowledge, this programme provides the solving and understanding capacity of major concepts in all disciplines of the chemistry independently

PO-2. Ability to communicate effectively in general and scientific topics with the scientific community and with society at large

PO-3. Well trained students face the employment challenges and inspire confidence to turn into entrepreneur and also step into research career

PO-4. Scientific temperament and research aptitude capability to ask relevant/appropriate questions for identifying, formulating and analyzing the research problems

PO-5. Individual and team work training impart to learn and work effectively as an individual and as a member or leader in diverse teams in multidisciplinary setup

PO-6. Techniques usage to learn skills in terms of modern tools for scientific practices

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PO-7. Ability to apply reasoning to assess the different issues related to society and the consequent responsibilities relevant to the professional scientific practices

PO-8. Capability to identify and apply ethical issues related to scientific work such as tempering the data, committing plagiarism and unbiased truthful actions

PO-9. Ability to demonstrate knowledge and understanding of the scientific principles and apply these to manage research work

PO-10. Ability to solving new chemical problems and to synthesize novel compounds and can predict reaction mechanism

Program Specific Outcomes (PSOs)

The program specific outcomes (PSO's) are the statement of skill/competencies/abilities that narrate the knowledge and capabilities at post-graduate level. To aware the recent frontier areas of knowledge and the tools/techniques/methodologies those are highly desirable for cutting edge research and solution of societal need. After successful completion of M. Sc. (Chemistry), the students will be able to

PSO-1. Understand the importance of various elements present in the periodic table and its abundance in the earth crust. Extraction/separation and purification of compounds/minerals can be done by using theories and instrumental knowledge.

PSO-2. Understand the detailed functional knowledge of theoretical concepts and experimental aspects of chemistry.

PSO-3. Explore the potential uses of analytical, industrial chemistry, polymer chemistry and medicinal chemistry.

PSO-5. To understand, analyze, plan and implement qualitative as well as quantitative analytical synthetic and phenomenon-based problems in chemical sciences.

PSO-6. Through separation/purification and natural product chemistry knowledge and skill that can crate own entrepreneurship that impart in ATMNIRBHAR mission.

PSO-7. Provide opportunities to excel in competitive exams, academics, research and industry.

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M.Sc. Chemistry Programme Structure

Year	Semester	Course Credit	No. of Course*
4	VII#	28	4 Core course 1 Minor elective course 1 Practical Course 1 Research Course
	VIII	24	4 Core course 1 Practical Course 1 Research Course
5	IX	24	4 Theory course (1 Core Course + 2 Specialization Course + 1 Elective Course) 1 Practical Course 1 Research Course
	X	24	4 Theory course (3 Specialization Course + 1 Elective Course) 1 Practical Course 1 Research Course
	Total	**100**	

***Credit of each theory, practical and research course is 4.**

1 Credit = 1 hr. per week for theory course

1 Credit = 2 hr. per week for practical and research course

- A 4 credit **theory course** will have four Lectures/periods (of one hour) in a week. In one full semester the course will be covered in 60 Lectures.
- A 4 credit **practical/project course** will have four lab periods (of two hours each) in a week. In one full semester the course will be covered in 60 Lab periods (120 hours)

According to NEP curriculum, the I, II, III & IV semester of Master programme will be VII, VIII, IX, and X which is in continuation of bachelor programme of six semester viz., I, II, III, IV, V, and VI,. Similarly, year 1 and 2 of Master programme will be year 4 and 5 which is in continuation of bachelor programme of three year viz., year 1, 2 and 3.

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The Full Structure and Scheme of the Semester Courses for the M.Sc. Chemistry

Subject Code	Title	Teaching Hours per week			Maximum Marks			Credits
		L	T	P	Sessional Marks	End-semester Examination	Total Marks	
SEMESTER VII								
B020701T	Coordination Chemistry	3	1	0	25	75	100	4
B020702T	Stereochemistry and Organic Reaction Mechanism	3	1	0	25	75	100	4
B020703T	Thermodynamics and Fast Kinetic Reactions	3	1	0	25	75	100	4
B020704T	Analytical Chemistry	3	1	0	25	75	100	4
B020705P	Chemistry Practical-I	0	0	12	25	75	100	4
B020706R	Fundamentals of Research [$]	0	0	12	-	-	100	4
	Minor Elective (to be opted from other department/Faculty)						100	4
Total							**700**	**28**
SEMESTER VIII								
B020801T	Molecular symmetry and electronic spectra	3	1	0	25	75	100	4
B020802T	Organic reaction and Pericyclic	3	1	0	25	75	100	4
B020803T	Quantum Chemistry and Photochemical Reactions	3	1	0	25	75	100	4
B020804T	Spectroscopy I	3	1	0	25	75	100	4
B020805P	Chemistry Practical II	0	0	12	25	75	100	4
B020806R	Research Proposal and Literature Survey[$]	0	0	12	-	-	100	4
Total							**600**	**24**
SEMESTER IX								
B020901T	Spectroscopy II	3	1	0	25	75	100	4
B020902T B020904T B020906T	***Specialization Course I**** Bioinorganic Rearrangements and photochemistry Gaseous state and Statistical Thermodynamics	3	1	0	25	75	100	4
B020903T B020905T B020907T	***Specialization Course II**** Organometallic Oxidation, reduction and organometallic reagents Magnetization and Irreversible Thermodynamics	3	1	0	25	75	100	4
B020908T B020909T B020910T	***Elective Course***** Environmental Chemistry Analytical Techniques Computational Chemistry	3	1	0	25	75	100	4
B020911P B020912P B020913P	***Lab Course******* Inorganic Chemistry Practical-I Organic Chemistry Practical-I Physical Chemistry Practical-I	0	0	12	25	75	100	4
B020914R	Experiment, Result & Discussion[$]	0	0	12	-	-	100	4
Total							**600**	**24**
SEMESTER X								
B021001T B021004T B021007T	***Specialization Course I*** [#] Coordination Polymers, Cages, Clusters & Nanostructures Biosynthesis and chemistry of natural products Solution and Advanced Quantum Chemistry	3	1	0	25	75	100	4
B021002T B021005T B021008T	***Specialization Course II*** [#] Main group and inner-transition elements Carbohydrates and vitamins Solids and Advanced Electrochemistry	3	1	0	25	75	100	4
B021003T B021006T B021009T	***Specialization Course III*** [#] Solid State and Nuclear chemistry Biomolecules Polymer Chemistry	3	1	0	25	75	100	4
B021010T B021011T B021012T	***Elective Paper*** [##] Reagents and reactions Supramolecular Chemistry Medicinal & Pharmaceutical Chemistry	3	1	0	25	75	100	4
B021013P B021014P B021015P	***Lab Course*** [###] Inorganic Chemistry Practical-II Organic Chemistry Practical-II Physical Chemistry Practical-II	0	0	12	25	75	100	4
B021014R	Research Project Report /Thesis[$]	0	0	12	-	-	100	4
Total							**600**	**24**
Grand Total							**2500**	**100**

Note:

$ Each student has to carry out a research project throughout the all four semester. The purpose of the dissertation in all semester is to introduce research methodology to the students. It may consist of review of some research papers, development of a laboratory experiment, fabrication of a device, working out some problem related to subject, participation in some ongoing research activity, analysis of data, etc. The work can be carried out in any thrust areas of subject (Experimental or Theoretical) under the guidance of allotted supervisor of the department. The students must submit their dissertation in the department as per the date announced for the submission. Internal assessment of the dissertation work will be carried out by respective supervisor through power point presentation given by candidates during the semester. External assessment of the dissertation work will be carried out by an external examiner (nominated by the Chairperson of the Department) through power-point presentation given by candidates. This load (equivalent to 2 hours per week) will be counted towards the normal teaching load of the teacher.

For IXth Semester

* opt two specialization course from specialization course I & II in combination of following; for

Inorganic specialization
B020902T Bioinorganic
B020903T Organometallic

Organic specialization
B020904T Rearrangements and photochemistry
B020905T Oxidation, reduction and organometallic reagents

Physical specialization
B020906T Gaseous state and Statistical Thermodynamics
B020907T Magnetization and irreversible thermodynamics

** *opt any one elective paper*

*** *opt one practical course according to the specialization course*

For Xth Semester

opt three specialization course from specialization course I, II & III in combination as follows

Inorganic specialization
B021001T Coordination Polymers, Cages, Clusters & Nanostructures
B021002T Main group and inner-transition elements
B021003T Solid State and Nuclear chemistry

Organic specialization
B021004T Biosynthesis and chemistry of natural products
B021005T Carbohydrates and vitamins
B021006T Biomolecules

Physical specialization
B021007T solution and advanced quantum chemistry
B021008T Solid and advanced electrochemistry
B021009T Polymer Chemistry

opt any one elective course

opt one practical course according to the specialization course

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Semester VII

Course Code: B020701T **Course Credit: 4; 60 hrs.**

Course Title: Coordination Chemistry

UNIT- I

Metal – Ligand Bonding in Transition Metal Complexes **15 hrs.**

Crystal field effect: Splitting of d orbital in Octahedral, Tetrahedral and Square planner symmetry; Crystal Field Stabilization Energy; Jahn-Teller distortions, Experimental evidence for covalency.

UNIT - II

Molecular orbital theory **10 hrs.**

Molecular orbital theory and its applications to metal complexes of octahedral, tetrahedral and square planner geometry.

UNIT-III

Reaction Mechanism of Transition Metal Complexes I **15 hrs.**

Inert and labile complexes, Stability Constant, Mechanism of octahedral substitution, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct indirect evidence in favor of conjugate mechanism.

UNIT-IV

Reaction Mechanism of Transition Metal Complexes II **10 hrs.**

Anation reactions, reactions without metal ligand bond cleavage, Substitution reactions in square planer complexes, the trans effect, mechanism of the substitution reaction.

UNIT-V

Reaction Mechanism of Transition Metal Complexes III **10 hrs**

Redox reactions, electron transfer reactions, mechanism of one electron transfer reactions, outer-sphere type reactions, cross reactions and Marcus-Hush theory, inner sphere type reactions.

Course outcomes (COs): After completing this course, the students will be able to understand:

CO-1: Metal-ligand bonding in coordination complexes
CO-2: Crystal field theory and molecular orbital theory
CO-3: Substitution reaction in coordination complexes
CO-4: Redox reaction
CO-5: Electron transfer reaction

Recommended Books:

1. James E. Huheey, Inorganic Chemistry:Principles of structure and reactivity
2. Gary L. Miessler, Inorganic Chemistry
3. Asim K Das, Fundamental concepts of inorganic Chemistry Vol. 4
4. B.R. Puri, L.R. Sharma, K.C. Kalia, Principles of Inorganic Chemistry
5. Kettle. S. F. A. Physical Inorganic Chemistry: A Coordination Chemistry Approach, Springer, Berlin, Heidelberg (1996).
6. B.N. Figgis, M.A. Hitchman, Ligand Field Theory and Its Applications, Willey, New York, 2000

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Course Code: B020702T **Course Credit: 4; 60 hrs.**

Course Title: Stereochemistry and Organic Reaction Mechanism

UNIT – I

Aromaticity and π-Molecular Orbitals of Conjugated Systems

Aromaticity and Huckel's rule (energy, structural, electronic criteria for aromaticity and relationship among them, aromaticity for annulenes, charged rings, homoaromaticity, fused rings, heteroaromaticiy).

Supramolecular chemistry: Host-guest systems, Crown ether complexes and cryptands, cyclodextrins, catenanes and rotaxane.

Reaction Mechanism: structure and reactivity

Thermodynamics and kinetics: Acids and bases, HSAB principle, bond energies and thermochemistry, kinetic parameters, Hammond's postulate, Kinetic isotope effects, kinetic and thermodynamic control (general relationship between thermodynamic stability and reaction rate). Linear free energy relationships for substituent effects

UNIT – II

Stereochemistry

Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, optical purity, enantiotopic and diasterotopic atoms, group and faces, stereospecific and stereoslective synthesis, Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape, R/S Nomenclature, chiral centers and chiral molecules. Conformational analysis of cycloalkanes, disubstituted cyclohexanes, decalin, effect of conformation on reactivity.

UNIT – III

Aliphatic Nucleophilic Substitution

The SN2, SN1, mixed SN1', SN2', SNi and SET mechanisms, The neighbouring group mechanism, neighbouring group participation (anchimeric assistance) by oxygen, halogen and sulpher as a neighbouring group.

Nucleophilic substitution at an allylic, aliphatic trigonal and vinylic carbon, reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis, ambident nucleophile and regioselectivity.

UNIT – IV

Aromatic Electrophilic Substitution

The arenium ion mechanism, orientation and reactivity, energy-profile diagrams. The ortho/para ratio, ipso attack. Diazonium coupling Vilsmeier-Haack reaction, Gatterman-Koch reaction. Generation, structure, stability and reactivity of nucleophilic carbenes, carbanion (enolateion), nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangement

UNIT – V

Aromatic Nucleophilic Substitution

The ArSN1, ArSN2 and benzyne mechanisms, Reactivity-effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser and Smiles rearrangements.

Course Outcome: After the completion of the course, the students will be able to understand:

CO-1: aromaticity, nonaromaticity and antiaromaticity in carbocyclic and heterocyclic compounds.

CO-2: mechanism and outcome of aliphatic electrophilic substitution reactions.

CO-3: properties and reactivity of stereoisomers and stability of an organic molecule based on structure, including conformation and stereochemistry, Conformational analysis and its effect on organic reactivity, stereoselective and stereospecific synthesis.

CO-4: the various types of aliphatic nucleophilic substitution reactions and will give them a better understanding of the processes involved.
CO-5: mechanisms for various organic reactions and how to use their understanding of organic mechanisms to predict the outcome of reactions.

Recommended books

1. Stereochemistry of Organic Compounds, Nasipuri, New Age International (P) Limited.
2. Stereochemistry of Carbon Compounds, E. L. Eliel and S. H. Wilen
3. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
4. Advanced Organic Chemistry, A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
5. Advanced Organic Chemistry, J. March, 6th Ed.
6. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
8. Advance Organnic Chemistry, Jagdamba Singh and L. D. S. Yadav, Pragati Publication
9. Guidebook to Mechanism in Organic Chemistry, Orient Longman, Sykes, P. A New Delhi.

SUGGESTED WEB SOURCES:

1. https://nptel.ac.in/course.html
2. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5
3. https://swayam.gov.in/explorer?category=Chemistry

Course Code: B020703T **Course Credit: 4; 60 hrs.**

Course Title: Thermodynamics and Fast Kinetic Reactions

UNIT – I

Partial Molar Properties, Nernst Heat Theorem (NHT) and Third Law of Thermodynamics

Partial molar properties, chemical potential, chemical potential and other thermodynamic functions, fugacity of real gases, Nernst heat theorem and its application to non-condensed systems, Statements of the third law of thermodynamics, Derivation of unattainability of absolute zero, The relationship between entropy constant and Nernst chemical constant, Determination of entropy from the third law using the correction due to gas imperfections.

UNIT – II

Statistical Mechanics

Quantum states and complexions, The combinatory rule, System with definite total energy, Degeneracy of energy levels, Probability and most probable distribution, Indistinguishability, Maxwell-Boltzmann statistics, partition function, Translational, rotational, vibrational, nuclear and electronic partition functions, Internal energy and heat capacity in terms of partition function.

UNIT – III

Quantum theory of Raman Spectra, Stokes and Anti-stokes lines, Rotation and vibration Raman spectra, Mutual exclusion principle, Laser Raman spectra, Theory of NMR relaxation process and chemical shift, The coupling constant, Nuclear spin interaction, Principle of ESR, Magnetic moment of electron and splitting factor, Hyper-fine splitting and double resonance in ESR.

UNIT – IV

Spectroscopy

Molecular Spectra- Basic concepts of molecular spectroscopy, Classification of spectra, Characterization of electromagnetic radiations, Regions of the spectrum,

Rotation Spectra- Rigid and non-rigid rotation spectra-selection rule, Centrifugal distortion, Isotopic shift, Spectra of polyatomic molecules, Rotational constant, Experimental techniques.

Vibration rotation spectra- Simple harmonic oscillator, Vibrational energy, Anhormonicity, principle of vibration-rotation spectra, selection rule, PQR branches, Vibration in polyatomic molecules, Effect of nuclear spin, Isotopic shift, group frequency, Experimental techniques.

Unit V

Kinetics of fast reactions: Techniques of study of fast reactions with reference to stop flow, T-Jump, Flash photolysis and relaxation phenomena. Kinetics of oscillating reactions with special reference to Belousov-Zhabotinskii mechanism (B-Z mechanism).

Course Outcomes: After completing this course, the students will be able to understand:

CO-1: Application of classical thermodynamics.
CO-2: Theories of statistical thermodynamics.
CO-3: Interaction of electromagnetic radiation with matter.
CO-4: Basic principles of IR, Raman, Microwave, NMR and ESR spectroscopy.
CO-5: Molecular Spectra, Rotation Spectra and Vibration rotation spectra
CO-6: Various methods for studying the kinetics of fast reactions.

Recommended books:

1. P.W. Atkins, Physical Chemistry,Oxford University press, New York.
2. Colin N. Banwell, Fundamentals of Molecular spectroscopy, McGraw - Hill book company.
3. R.S.Drago, Physical methods in Chemistry, New age publication, New Delhi.
4. K.L.Kapoor, Advance Physical Chemistry (Vol. 1,2,3,4), MacMillan, India.

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5. I.N. Levine, Quantum Chemistry.
6. Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar
7. M.C.Gupta, Statistical Thermodynamics, New Age International Limited Publisher, India.
8. R.Chang. Basic principles and spectroscopy, Mcgraw Hill Publishing company Limited, India.
9. A.K.Chandra, Introductory Quantum Chemistry,Mcgraw Hill Publishing company Limited, India.

Course Code: B020704T **Course Credit: 4; 60 hrs.**

Course Title: Analytical Chemistry

Unit I

Characteristics of an analysis: Classification of errors and their minimization, standard deviation, Normal error curve. Statistical Tools: Population vs. Sample, Mean standard Deviation and variance, Confidence Limits, Analyzing data sets identifying outliers: The Q-Test, Linear regression analysis.

Unit II

Quantitative Calculations: Principle, applications and limitations of spectrophotometery. The Lambert-Beer's Law; Mixtures of absorbing species-laws of additivity of absorbance; calibration curve for calculation of unknown; Spectrometric errors in measurement; Deviation from Lambert-Beer's law-chemical deviation,

Unit III

Potentiometry

General principles, calomel electrodes, Ag/AgCl electrodes, membrane electrodes, ion selective electrodes, glass electrodes, liquid membrane electrodes.

Unit IV

Separation Methods-I: General principle, Classification of chromatographic methods: adsorption chromatography, partition chromatography, size exclusion chromatography, ion exchange chromatography, affinity chromatography. Nature of partition forces. Chromatographic behaviour of components. Distribution Coefficient, Rf value, Retardation, Retention, Capacity factor, Separation factor, Column efficiency and resolution. Van Deemter equation. Thin layer chromatography: Solvents used in methods of detection.

UNIT- V

Separation Methods-II: Column chromatography: Adsorption and partition methods. Nature of column materials. HPLC: Principle and Instrumentation, general components of a high performance liquid chromatography, solvent delivery systems, sample injection system, HPLC detectors. Hyphenated techniques: LC-MS.

Course outcome: After completing this course, the students will be able to understand:
CO-1: newer insight regarding big chemical data analysis and handling
CO-3: the concept of spectrophotometery and practical application
CO-4: theories and importance of Potentiometry
CO-5: general principles of separation technique.
CO-6: ideas of separation technique such as HPLC.

Recommended books:

1. G. D. Christian; Analytical Chemistry, John Wiley; 6 th Edition.
2. J.H. Kennedy, Analytical Chemistry: Principles, Saunders College Publishing, 2 nd Edition.
3. G. W. Ewing, Instrumental Methods of Chemical Analysis, McGrawHill Int 5 th Ed.
5. D. A. Skoog, D.M. West, F.J. Hollar, S.R. Crouch; Fundamentals of Analytical Chemistry, Cengage learning; 9 Ed.
6. J. Mendham, R.C. Denney, J.D. Barnes and M. Thomas; Vogel's Textbook of Quantitative Inorganic Analysis; 6 th Edition, Pearson Education Asia 2005
7. H. Willard, L.L. Merritt, J.A. Dean, F.A. Settle, Instrumental methods of Analysis; HCBS Publishing New Delhi; 2004, 7th Ed.

Course Code: B020705P **Course Credit: 4; 120 hrs.**

Course Title: Chemistry Practical I

INORGANIC CHEMISTRY-I

Qualitative Analysis

Qualitative mixture analysis for seven radicals including two rare elements. (Mo, W, Ti, Zr, Th, Ce, V) in cationic and anionic forms.

Quantitative separation and determination of the following pairs of metal ions using gravimetric and volumetric methods

I. Ni^{2+} (gravimetrically) and Cu^{2+} (Volumetrically)
II. Ba^{2+} (gravimetrically) and Cu^{2+} (Volumetrically)
III. Fe^{3+} (gravimetrically) and Ca^{2+} (Volumetrically)
IV. Mg^{2+} (gravimetrically) and Ca^{2+} (Volumetrically)

ORGANIC CHEMISTRY-I

A. Separation and identification of organic compounds using chemical methods from binary mixtures. Use TLC for checking the purity of the separated compounds and their derivatives and report their R_f values.
B. Estimation of glucose, aldehydes and ketones by chemical and spectroscopic methods.

PHYSICAL CHEMISTRY-I

1. Kinetic studies of a reaction between acetone and iodine catalysed by H^+ ions
2. Kinetics of oxidation of reducing sugars by potassium ferricyanide in presence of ammonium hydroxide or sodium hydroxide
3. Potentiometric titration of strong acid and strong base.
4. Determination of total dissolves solids in tap water.
5. Determination of Rf value with help of paper chromatography
6. Determination of percentage composition of two miscible liquid using stalagmometer

Course Outcome: After completing this course, the students will be able to understand:

CO-1. qualitative analysis of inorganic mixtures and insolubles.
CO-2. separation techniques of cations and anions by chromatography.
CO-3. qualitative analysis of three component organic mixture.
CO-4. the basic knowledge like preparation of solutions standardization of secondarysolution, dilution, calibration and handling of some sophisticated electronic relatedto the practical syllabus.
CO-5. the basic knowledge of conductance, e.m.f, pH, kinetics and partition coefficient.
CO-6. to focus their aim for future prospects of Ph.D. programme and Pharmaceutical industry.

Recommended Book:

1. The systematic Indentification of Organic Compounds, R.L. Shringer and D.Y. Curlin.
2. Qualitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
3. Basic concept of Analysis chemistry, S.M. Chopkar, Wiley Bastern.
4. Systematic Qualitative Organic Analysis, H. Middeton, AdwardArnoid.
5. Handbook of Organic Analysis Qualitative and Quantitative, H. Clark, Adward Ar.
6. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
7. General Chemistry Experiments, Anil J Elias, University Press (2002)

Course Code: B020706R **Course Credit: 4; 60 hrs.**

Research Course Title: Fundamental of Research

UNIT – I

Introduction to research **12 hrs.**

Objectives, research ethics, Identification of emerging research area, selection of research topic, feasibility of research topic,

UNIT – II

Computer and internet in research: **12 hrs.**

Computer, internet, search engines, MS office etc

UNIT – III

Packages and software for Chemistry research **12 hrs.**

Chem Draw, Origin, Gaussian and other related software

UNIT – IV

Literature review, publication, IPR and patent **12 hrs.**

Literature review, manuscript preparation, scientific journals, research article, review article, publication process, peer review, intellectual property rights, patents

UNIT – V

Project proposal, Manuscript and thesis writing **12 hrs.**

Project proposal, synopsis, thesis writing,bibliography,plagiarism, copyrights.

Course outcomes: After completing the course, students will be able to

- understand the basic idea of research
- identify research area for their project
- write proposal, synopsis and dissertation
- use soft skills for research purpose
- understand publication & patent process, plagiarism, IPR

Course Code: As per other department course code **Course Credit: 4; 60 hrs.**

Course Title: Minor Elective*

(*opted from other department/faculty)

Semester VIII

Course Code: B020801T **Course Credit: 4; 60hrs.**

Course Title: Molecular Symmetry and Electronic Spectra

UNIT – I

Introduction to Molecular Symmetry **12 hrs.**

Symmetry and group theory, symmetry operations, symmetry elements: axis of symmetry, plane of symmetry, improper rotational axis, inversion centre and identity, identification of different symmetry elements in inorganic molecules.

UNIT – II

Molecular Point Groups **12 hrs.**

Point Groups, identification of molecular point groups, molecule of low, high and special symmetry, symmetry and point group consideration in simple inorganic and coordination compounds.

Unit-III

Character Table **12 hrs.**

Groups,subgroups, classes, group multiplication table of C_{2v}& C_{3v}, character of an operation, orthogonality, reducible and irreducible representations,character tables and its application in infrared and Raman spectroscopy

Unit-IV

Terms and States for Electronic Spectroscopy **12 hrs.**

Frank – Condon principle, spin and Laporte selection rules, band intensities, band-width, number of microstates and term symbols for gaseous atoms/ions.spin-orbit coupling in spectroscopic ground state of p^2 and d^2 configurations and energies of J levels.

UNIT-V

Electronic Spectra of Transition Metal Complexes **12 hrs.**

Interpretation of electronic spectra usingOrgel and Tanabe – Sugano diagram for 3d transition metal complexes, calculations of crystal field and ligand field parameters (Dq, B and ß parameters), nephelauxetic series and charge transfer spectra.

Course outcomes (COs): After completing the course, students will be able to:

CO-1 understand basic concept symmetry in chemical molecule
CO-2 identify different symmetry element and point group of molecules
CO-3 understand application of symmetry in spectroscopic investigation
CO-4 understand different electronic state and electronic transition in molecule

Recommended Books

1. K. Veera Reddy, Symmetry and Spectroscopy of Molecules, New Age Inter Pvt. Ltd., New Delhi, 1999.
2. Allan Vincent, Molecular Symmetry and Group Theory. John Wiley & Sons, LTD.
3. R. McWeeny, Dover Publications,Inc.Symmetry: An introduction to group theory and its applications.
4. F. A. Cotton, Chemical Applications of Group Theory. John Wiley & Sons, Inc.
5. S. F. A. Kettle, Symmetry and Structure. Wiley
6. Sutton, Electronics Spectra of Transition Metal Complexes, Mc-Graw-Hill, London, 1968.

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Course Code: B020802T **Course Credit: 4; 60 hrs.**

Course Title: Organic Chemistry

UNIT-I

Free Radical Reactions **12 hrs.**

Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes, Free radical rearrangement, Hunsdiecker reaction.

Addition to carbon-carbon Multiple Bonds

Mechanistic and stereochemical aspect of addition reaction involving electrophiles, nucleophiles and free radicals, regio and chemoselectivity, orientation and reactivity. Hydroboration, Michael reaction, Sharpless asymmetric epoxidation, Stereochemistry of epoxidation.

UNIT-II

Addition to Carbon-Hetero atom Multiple Bonds **12 hrs.**

Generation of enolate ions and their Synthetic applications. Stereochemistry of Witting reaction and Aldol condensation. Stobbe condensation reactions. Hydrolysis of esters.

Elimination Reactions The E_2, E_1 and E_1cB mechanisms and their stereochemistry and orientation. Reactivity-effects of substrates, attacking base, the leaving group and the medium. Mechanism and orientation in pyrolytic elimination and Paterson elimination.

UNIT-III **12 hrs.**

Pericyclic Reactions Molecular orbital symmetry, Frontier orbitals of ethylene, 1, 3-butadiene, 1.3,5-hexatriene and allyl system, Classification of pericyclic reactions, Woodward-Hoffmann correlation diagrams, FMO and PMO approach, Electrocyclic reactions-conrotatory and disrotatory motions, 4n, 4n+2 and allyl systems.

UNIT-IV **12 hrs.**

Cycloadditions-antrafacial and suprafacial additions, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3-dipolor cycloadditions and cheleoptropicrections

UNIT-V

Sigmatropic rearrangement **12 hrs**

Suprafacial and antarafacial shift of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, (3,3) and (5,5) sigmatropic rearrangements, detailed treatment of Claisen and Cope-rearrangements. Fluxional tautomerism, Aza-Cope rearrangements. Introduction to Ene reactions. Simple problems on pericyclic reactions.

Course Outcome: After completing the course, students will be able to understand:

CO-1: aromatic electrophilic and nucleophilic substitutions and their mechanism

CO-2: free radical reactions, their mechanism and also the reactivity towards aliphatic and aromatic

CO-3: addition reactions between carbon- carbon multiple bonds and hetero atom and carbon multiple bonds and mechanism of some specific name reactions.

CO-4: elimination reactions and rules used to study elimination reactions with the help of specific examples of elimination reactions.

CO-5: molecular orbital symmetry and possibility of thermal and photochemical pericyclic reactions.

Recommended Books

1. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
2. Advanced Organic Chemistry, A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
3. Advanced Organic Chemistry, J. March, 6th Ed.
5. Advance Organnic Chemistry, Jagdamba Singh and L. D. S. Yadav, Pragati Publication
6. Textbook of Pericyclic Reaction, Concept and Application, K.C. Majumdar and P. Biswas, Scientific International Pvt. Ltd.
7. Photochemistry and Pericyclic Reactions, Jagdamba Singh and Jaya Singh, New Age International

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Course Code: B020803T **Course Credit: 4; 60 hrs.**

Course Title: Quantum and Photochemical Reactions

UNIT-I

12hrs.

Quantum Chemistry

Postulates of quantum mechanics, Three dimensional time independent Schrodinger wave equation, Eigen functions and eigen values, Normalization and orthogonality conditions, One dimensional harmonic oscillator, Tunnel effect, Eigen function and eigen value of H-atom (Solutions not required), Radial and Angular distribution curves for He-atom shapes of s, p, d and f- orbitals

Approximate Methods- Variation principle and its application to ground state H-atom.

UNIT-II

12hrs.

Chemical Kinetics

Thermodynamic formulation of rate constant, Comparison of collision and absolute reaction rate theories, Calculation of transmission coefficient, Transition State Theory in Solution, Primary and Secondary salt effects in the light of mechanistic tests, The theory of Absolute reaction rates for reactions between atoms and reactions between molecules in terms of partition function, Influence of ionic strength and dielectric constant, Explosive reactions.

UNIT- III

12hrs.

Photochemical reactions

Absorption of light, chain reactions, free radical chains (Rice-Herzfield mechanism for the decomposition of ethane), Lambert's and Beer's law, Grotthus Draper law,Einstein's law of photochemical equivalence , Quantum efficiency , Reasons for low and high quantum yields , Kinetics of some typical photochemical reactions (decomposition of acetaldehyde , Dimerisation of anthracene etc.), Photoelectric cell , Photosenstization.

UNIT-IV

12hrs.

Electrolytes

Limitation of Arrhenius theory of electrolytic dissociation, Role of solvent and inter-ionic forces, activities and activity coefficients, determination of activity coefficients, Debye-Huckel Theory of the structure of dilute ionic solution, charge density and electrical potential, Properties of ionic cloud, activity coefficients from Debye-Huckel theory, Limiting law and its verification, Debye-Huckel Theory to more concentrated solutions, Partial molar quantities of electrolytic solutions, determination of partial molar volume.

UNIT- V

12hrs.

Intermolecular forces

Nature of intermolecular forces, Various contributions of intermolecular forces, London theory of dispersion forces, Intermolecular potentials for polar and non-polar molecules, Potential parameters of L-J potential and evaluation of second virial coefficients. Partition function of imperfect gas and Virial equation of State, Critical constants and L-J parameter.

Course Outcomes: After completing this course, the students will be able to understand:

CO-1: Schrodinger wave equation,1-D harmonic oscillator and tunnel effect.

CO-2: The connection between common approximation methods and standard chemical framework, e.g., Born-Oppenheimer approximation.

CO-3: The factors affecting the rate of a chemical reactions and the theoretical basis of rate determination.

CO-4: The various photo-physical and photochemical processes occurring after absorption of UV-Visible radiation.

CO-5: The various eventstaking place during and after electrolysis.

CO-6: The various types of forces present among molecules and atoms and, their genesis.

Recommended books:

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1. P.W. Atkins, Physical Chemistry,Oxford University press, New York.
2. S.Glasstone, An introduction to Electrochemistry, D. Van Nostrand company Inc..
3. K.L.Kapoor, Advance Physical Chemistry (Vol. 1,2,3,4), MacMillan, India.
4. I.N. Levine, Quantum Chemistry.
5. Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar Punjab.
6. Keith J.Laidler, Chemical Kinetics, Pearson Education Publisher.
7. Santosh K.Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer.
8. V.K.Thankappan, Quantum Mechanics through Problems, New Age International Publishers, New Delhi.
9. K.K.Rohatgi- Mukherjee, Fundamentals of Photochemistry,New Age International Publishers, New Delhi.
10. R.K.Prasad, Quantum Chemistry, New Age International Publishers, New Delhi.

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Course Code: B020804T **Course Credit: 4; 60 hrs.**

Course Title: SPECTROSCOPY

UNIT-I

Ultraviolet and Visible Spectroscopy: **10hrs.**

Various electronic transitions (185-800 nm), Beer-Lambert Law, effect of solvent on electronic transitions, ultraviolet bands for unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and unsaturated carbonyl compounds. Steric effect in biphenyls.

UNIT-II

IR and Raman Spectroscopy **10hrs.**

IR-Spectroscopy: Basic Principles characteristic frequencies of common functionalgroups, application to organic and inorganic compounds. Raman Spectroscopy: Classical theories of Raman effect, Pure vibrational, vibrational-rotational Raman spectra, Selection rule, mutual exclusion principle, Surface-enhanced Raman scattering.

UNIT-III

NMR spectroscopy **15hrs.**

General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), chemical exchange, effect of deuteration factor influencing coupling constant 'J'. Spin decoupling, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), virtual coupling. Stereochemistry, hindered rotation, Karplus curve-variation of coupling constant with dihedral angle. Simplification of complex spectra-nuclear magnetic double resonance, contact shift reagents, solvent effects. Fourier transform technique, nuclear Overhauser effect (NOE). advantage of FT NMR, use of NMR in medical diagnostics.

UNIT –IV **10hrs.**

Two dimension NMR spectroscopy: Introduction to COSY and DEPT techniques; Nuclear quadrupole resonance spectroscopy: Quadrupole nuclei, quadrupole moments, electric field gradient, coupling constant, splitting; Carbon-13 NMR Spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants.

UNIT-V

Mass spectrometry **10hrs.**

Basic principles, ionization techniques, isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution MS, soft ionization methods, ESI-MS and MALDI-MS, illustrative examples from macromolecules and supramolecules.

Applications of IR, NMR and Mass spectroscopy for structure elucidation of organic compounds

Course Outcomes: After completing this course, the students will be able to understand:

CO-1: UV-Vis spectroscopy and their application for characterization

CO-2: principle and application of IR and RAMAN

CO-3: NMR spectroscopy and different related phenomena

CO-4: use of NMR spectroscopy in in characterization of organic compounds

CO-5: basic principle and application of Mass spectrometry

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Recommended books:

1. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
2. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
3. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, McGraw Hill, 6th edition 2007.
4. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012.
5. H. Gunther, NMR Spectroscopy Wiley-VCH, 2013.
6. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.
7. L.D.S Yadav, Organic Spectroscopy, Kluwer academic publisher

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Course Code: B020805P **Course Credit: 4; 120 hrs.**

Course Title: Chemistry Practical - II

INORGANIC CHEMISTRY

1. Preparation of following coordination complexes and their characterization by m.p, elemental analysis and molar conductivity measurements
   $[Cu(NH_3)_4]$; $K_3[Cr(C_2O_4)_3].3H_2O$; $Mn(acac)_3$, $[Co(Py)_2Cl_2]$; $Na[Cr(NH_3)_2(SCN)_4]$; $K_3[Fe(C_2O_4)_3]$; $[Ni(NH)_6]Cl_2$; $Hg[Co(SCN)_4]$; $VO(acac)_2$

2. Study of recorded UV-visible and IR of above prepared coordination compounds.

ORGANIC CHEMISTRY

1. Preparation of various organic compounds involving two or three steps employing different reactions viz. Aldol Condensation, reactions of enolate ions, oxidation rections, Cannizzarro reaction, Molecular rearrangement reactions etc. with a view to give the student sufficient synthetic training in synthetic organic chemistry
2. Isolation of Caffeine from tea leaves and Eugenol from clove

PHYSICAL CHEMISTRY

1. Kinetics of reaction between $K_2S_2O_8$ and KI.
2. Analysis of a mixture of sucrose, fructose and dextrose by Polarimeter.
3. Determination of CMC (critical micellization conc.) by conductometrically.
4. Determination of percentage composition of two miscible liquid using viscometer.

Course Outcomes: After completing this course, the students will be able to understand:

CO-1. preparation of coordination compound
CO-2. Characterization by UV-Vis spectroscopy
CO-3. Extraction and separation of organic compounds
CO-4. the basic knowledge and handling of the conductometer
CO-5. the basic knowledge and handling of polarimeter

Recommended Book:

1. The systematic Indentification of Organic Compounds, R.L. Shringer and D.Y. Curlin.
2. Qualitative Analysis, R.A. Day, Jr. and A.L. Underwood, Prentice Hall.
3. Basic concept of Analysis chemistry, S.M. Chopkar, Wiley Bastern.
4. Systematic Qualitative Organic Analysis, H. Middeton, AdwardArnoid.
5. Handbook of Organic Analysis Qualitative and Quantitative, H. Clark, Adward Ar.
6. Vogel's Textbook of Practical Organic Chemistry, A.R. Tatchell, John Wiley.
7. General Chemistry Experiments, Anil J Elias, University Press (2002)

Course Code: B020807R **Course Credit: 4; 120 hrs.**

Course Title: Research Proposal and Literature Survey

A topic of research project will be allotted to the students. For project work and dissertation, the area of the work would be to be decided by the advisor/mentor. Research proposal and literature survey will be done in this semester (VIIIth Sem.). At the end of the semester, students have to submit a report and present their findings and progress of the allotted research work. Student may also allow for summer internship or training (at least 60 to 90 days) will consider as equivalent to his/her project work. However, students have to submit a report and present their findings and progress of his/her summer internship or training.

SEMESTER IX

Course Code: B020901T **Course Credit: 4; 60 hrs.**

Course Title: Spectroscopy II

UNIT- I

Electron Spin Resonance Spectroscopy: Basic principle, Hyperfine Splitting (isotropic systems); the g value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Karamer's degeneracy); Electron-electron interactions, Anisotropic effects (the g value and the hyperfine couplings); Structural applications of transition metal complexes.

UNIT- II

Nuclear Spectroscopy – Multinuclear NMR of Metal nuclei. ^{31}P, ^{9}F, ^{27}Al, ^{11}B, ^{119}Sn and ^{51}V.

UNIT- III

Mossbauer Spectroscopy: Basic principle, conditions for Mossbauer spectroscopy, spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature dependent effects, structural deductions for iron and tin – complexes, miscellaneous applications. Nuclear Quadrupole Resonance (NQR) – Theory and its applications.

UNIT- IV

X-ray Photo electron Spectroscopy and Related Techniques: Basic principles, spectral features and their applications to structural determination of inorganic molecules and metal complexes: X-ray Photoelectron Spectroscopy (XPS), Auger Electron Spectroscopy (AES).

UNIT- V

Electron Microscopy

SEM (Scanning electron microscopy), and TEM (Transmission electron microscopy), AFM (Atomic force microscopy), STM (Surface tunneling microscopy).

Course Outcomes: After completing this course, the students will be able to understand:

CO-1: ESR spectroscopy and their application for characterization

CO-2: principle and application of multinuclear NMR

CO-3: X-ray Photo electron Spectroscopy and different related phenomena

CO-4: use electron microscopy in characterization of organic compounds

CO-5: basic principle and application of Mossbauer Spectroscopy

Recommended books:

1. R. M. Silverstein, F. X. Webster, D. J. Kiemle, Spectrometric identification of organic compounds, 7th edition, John Wiley, 2005.
2. Organic Spectroscopy, W. Kemp, 3rd edition, Macmillan, 2011.
3. D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, McGraw Hill, 6th edition 2007.
4. D. L. Pavia and G. M. Lampman Spectroscopy 4th Edition, Brooks Cole, 2012.
5. H. Gunther, NMR Spectroscopy Wiley-VCH, 2013.
6. P. S. Kalsi, Spectroscopy of Organic Compounds, 6th edition, New age international, 2004.
7. L.D.S Yadav, Organic Spectroscopy, Kluwer academic publisher

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Course Code: B020902T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Bioinorganic Chemistry

UNIT-I

Role of Metal Ions in Biological Systems: **10 hrs.**

Photosystems; nitrogen fixation, Na^+ / K^+ pump.

UNIT-II

Complexes of Biological Significance: **10 hrs.**

Metal complexes of porphyrins and phthalocyanin, Vitamin B_{12} and B_6; chloropyhylls.

UNIT-III

Metallo Proteins: **15 hrs.**

Function, Electronic structure, bonding and stereochemistry of the active site –

(1) Natural oxygen carring proteins – Haemoglobin, Myoglobin, Hemerythrins and Hemocyanin

(2) Electron Transport Protein – (a) Iron – sulfer Proteins – Rubredoxin and Ferrodoxins (b) Cytochromes (types a, b and c)

UNIT-IV

Metallo enzymes I: **15 hrs.**

Mo-containing Enzymes – Nitrogenase; Xanthine Oxidase, sulphite, Oxidase and Nitrate reductase (b) Iron-containing enzymes, cytochrome -c- oxidase, catalases, Peroxidases, cytochrome-p-450

UNIT-V

Metallo enzymes II: **10 hrs.**

Copper – containing Enzymes – Superoxide dismutase (SOD), Bovine Superoxide dismutase (BOD), ascorbic acid oxidase and (b) Zinc–containg Enzymes carboxy – peptidase A and B; carbonic anhydrase and Urease.

Course outcomes (COs): After completing the course, students will be able to:

CO-1: understand different types metal complexes of porphyrins and phthalocyanin

CO-2: function, electronic structure, bonding of metallo proteins

CO-3: understand different metallo enzymes

CO-4: biological application of metallo enzymes

Recommended Books

1. G. N. Mukherjee and A. Das Elements of Bioinorganic Chemistry.
2. Ajai Kumar, Organometallic & Bioinorganic Chemistry Paperback – 1 January 2021
3. M. N. Hughes, Inorganic Chemistry of Biological Processes, 2nd Ed.(1981), John-Wiley & Sons, New York.
4. W. Kaim and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York (1995)
5. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, (1994).

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Course Code: B020803T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Organometallic Chemistry

UNIT-I

Introduction to organometallic compounds **10 hrs.**

Definition and classification of organometallic compounds based on hapticity and polarity of M-C bond; Nomenclature and general characteristics; metal hydrides (classical and non-classical)

UNIT-II

Complexes of σ-Donar π -donor Organic Ligands **20 hrs.**

Preparation, bonding and structure of alkene, alkyne, allyl, arene, carbenes and carbyenes complexes, important reactions with special reference to nucleophilic and electrophilic attack on ligands and to organic synthesis.

UNIT-III

Organometallic reactions **10 hrs.**

Oxidative addition, reductive elimination, migratory insertion, β-hydride transfer reactions, C-H bond activation.

UNIT-IV

Organometallic compounds in Catalysis **10hrs.**

Waker Process, hydrocarbanylation of olefins, hydrogenation, hydroformylation and Zeigler-Natta polymerization of olefins,

UNIT-V

Fluxional Organometallic Compounds **10hrs.**

Fluxionalloy and dynamic equilibria in compounds such as n^2 – olefins and n^3 – allyl and dienyl complexes.

Course outcomes (COs): After completing the course, students will be able to:

CO-1: understand different organometallic compounds

CO-2: to understand different σ-Donar π -donor Organic ligand

CO-3: understand different organometallic compounds in catalysis

CO-4: biological application of fluxional organometallic compounds

Recommended Books

1. F.A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 6th Ed. (1999) John Wiley & Sons, NY.
2. B.D. Gupta, Anil J. Elias Basic Organometallic Chemistry: Concepts, Syntheses and Applications Paperback – 1 January 2010
3. J.E. Huheey, Keiter and Keiter, Inorganic Chemistry,
4. R. H. Crabtree, The Organometallic Chemistry of Transition Metals, John Wiley.
5. Ch. Elschenbroich and A. Salzer, Organometallics, VCH.
6. J.P. Collman, L.S. Hegedus, J.R. Norton and R.G. Finke, Principles and Applications of Organotransition metal Chemistry, Univ. Sci. Books, Mill Valley, California

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NCL 23-9-22

Course Code: B020904T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Rearrangements and Photochemistry

UNIT-I

Molecular Rearrangements: Migration to electron deficient carbon atom

General mechanistic considerations – nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements-Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzilic acid, Favorskii, Arndt-Eistert synthesis, Neber, Beckmann, Hofman, Curtius, Schimdt, Baeyer-Villiger, Shapiro reaction.

UNIT-II

Ionic liquids as Phase Transfer Catalysis – synthesis of ionic liquids, physical properties and applications in alkylation, hydroformylations, expoxidations, synthesis of ethers, Phase transfer catalyst - Synthesis and applications

Nano-Chemistry: Introduction to nano-chemistry, fullerenes, nanotubes, carbon nano-particles and graphene.

UNIT-III

Green chemistry: Basic Principle and need of green chemistry, atom economy, step economy, Different tools for green synthesis (Elementary idea of green reagent, green solvent, green catalyst, solid phase, mw and ultrasound assisted) atom economy, green synthesis of BHC.

UNIT-IV

Photochemistry I: Photochemical energy, Franck - Condon Principle, Jablonski diagram singlet and triplet states, dissipation of photochemical energy, photosensitization, quenching, quantum efficiency and quantum yield, experimental methods of photochemistry. Photochemistry of carbonyl compounds π-π^* and n- π^* transitions. Norrish type I and Norrish type II cleavages, Patterno-Buchi reaction. Photochemistry of enone, Hydrogen abstraction, - rearrangement α, β unsaturated ketones and cyclohexadienes, photochemistry of p-benzoquniones.

UNIT-V

Photochemistry II: Olefins, cis-trans isomerisation, dimerisation, hydrogen abstraction and additions. Acetylenes-dimerisation, Dienes-photochemistry of 1, 3-butadiene (2+2) additions leading to cage structures, photochemistry of cyclohexadienes, Photochemistry of aromatic compounds-exited state of benzene and its 1,2 and 1, 3-shifts, Photo-Fries rearrangement, Photo-Fries reaction of anilides, photosubstitution reaction of benzene derivatives, Photolysis of nitride esters and Barton reaction.

Course outcomes (COs): After completing the course, students will be able to:

CO-1: understand different types and distinctive features of advanced organic reactions such as rearrangement reactions

CO-2: understand different types and distinctive features of a Ionic liquids as Phase Transfer Catalysis

CO-3: understand different types and distinctive features of advanced organic reactions in Green chemistry:

CO-4: basics of photochemical reactions of alkenes, carbonyl and aromatic compounds

Recommended Books:

1. Introductory Photochemistry,.A. Cox and T. Camp McGraw Hill.
2. Problem Solving approach to Orbital Symmetry, R.E. Lehr and A.P. Merchand
3. Organic Synthesis, Pragati Edition, Jagdamba Singh and L.D.S Yadav.
4. Some modern methods of organic synthesis, W. Carruthers, Cambridge University Press.
5. Organic Reactions and Their Mechanisms, P. S. Kalsi, New Age Science.

Nil 23-9-22

6. Rohatgi-Mukherjee, Fundamentals of Photochemistry, Wiley-Eastern Ltd., New Delhi, 1978.
7. R. P. Wayne, Principles and Application of Photochemistry, Oxford University Press, 1988.
8. Jagdamba Singh, Jaya Singh, Photochemistry and Pericyclic Reactions, New Age International (P) Limited.
9. Organic Photochemistry: A visual approach, Jan Kopecky, VCH publishers (1992).
10. Oganic Photochemistry, O. Kan, McGraw-Hill Inc., US.
11. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press).

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Course Code: B020905T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Oxidation, Reduction and Organometallic Reagents

UNIT-I

Oxidation

Introduction. Different oxidative processes. Hydrocarbons-alkenes, aromatic rings, saturated C-H groups (activated and unactivated). Alcohols, diols, aldehydes, ketones, ketals and carboxyalic acids. Amines, hydrazines, and sulphides. Oxidations with ruthenium tetraoxide, iodobenzene diacetate and thallium (III) nitrate.

UNIT-II

Reduction

Introduction. Different reductive processes. Hydrocarbonsalkanes, alkenes, alkynes and aromatic rings. Carbonyl compounds-aldehydes, ketones, acids and their derivatives. Epoxides. Nitro, nitroso, azo and oxime groups.

UNIT-II

Chiral pool approach, Acyclic stereoselection: reactions at α-and β-positions of a chiral center. Auxillary econtrolled stereoselection: Evans oxazolidones, Oppolzer sultams, Myers amides, Enders RAMP/SAMP, Sholkopf. Enantioselective alkylation allylation and crotylation reactions Asymmetric oxidation [epoxidation (Sharpless, Jacobsen, Shi), dihydroxylation (Sharpless)], reduction (Noyori, Corey, Pfaltz)

UNIT-IV

Synthetic Strategies:

Synthetic Strategies for formation of carbon-carbon bond, carbon-nitrogen bond and carbon-halogen bond.

UNIT-V

Organometallic Reagents

Synthetic applications of organometallic compounds with mechanistic details of following metals, Hg, Cd, Ce, Cu, Ni, Fe, Co, Rh, Cr and Ti.

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

CO-1: understand different types and distinctive features of advanced organic reactions, catalysts and reagents

CO-2: understand the advanced concepts related to the structure and properties of various organic catalysts, reagents and compounds

CO-3: design new catalysts, new reagents, new green reactions and properties based on the fundamental insights received

CO-4: appreciate the advanced sustainable reactions, reagents and catalysts for revolutionary applications in modern chemical sciences

CO-5: understand the advanced concepts related to asymmetric synthesis

Recommended Books:

1. M. Nogrady, *Stereoselective Synthesis: A Practical Approach*, Wiley, 2008.
2. E. M. Carreira, L. Kvaerno *Classics in Stereoselective Synthesis*, Wiley-VCH: Weinheim, Germany, 2009.
3. K. C. Nicolaou, E. J. Sorenson, *Classics in Total Synthesis*, Wiley-VCH.
4. K. C. Nicolaou, S. A. Snyder, *Classics in Total Synthesis II*, Wiley-

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Course Code: B020906T **Course Credit: 4; 60 hrs.**

Course Title: Physical Chemistry (Gaseous State and Statistical Thermodynamics)

UNIT-I

Distribution law (Barometric formula), Sedimentation equilibrium, Maxwell's law of distribution of velocity and energy, Maxwell's law and Gaussian density function, R,M,S, Mean and Most probable velocities, Collision frequency, Collision between like and unlike molecules, Triple collision.

UNIT-II

Viscosity, Thermal conductivity and Diffusion coefficient of gases (quantitative treatment), Mean free path. Mean and standard deviation absolute and relative errors, Linear regression, covariance and correlation coefficient.

UNIT-III

Calculation of thermodynamic properties from spectroscopic data, Bose-Einstein statistics, Fermi Dirac Statistics, Comparison of M-B, B-E and F-D statistics, Fermi-Dirac gas (Electron gas in metals), Bose -Einstein gas (liquid Helium).

UNIT-IV

Indistinguishbility of gas molecules, Maxwell-Boltzmann law for gaseous system, Thermodynamic functions for gaseous systems, Molar heat capacity of gases, Heat capacity of hydrogen at low temperatures, Heat capacities of monoatomic crystals, The Einstein model, Debye's theory of solid, Heat capacities of crystals at very low temperatures.

UNIT-V

Calorimetric entropy, Spectroscopic entropy, Comparison of calorimetric and Spectroscopic entropies, Third law of thermodynamics (i) Nernst Heat Theorem (ii) Entropy of chemical reactions (iii) statements of third law of thermodynamics and (iv) Conventional entropies, Expression of equilibrium constant in terms of partition functions, Equilibrium constants of simple system-(i) Ionization of metal atoms, (ii) Dissociation of diatomic molecules and (iii) Isotopic exchange equilibria.

Course Outcomes:

After completing this course, the students will be able to learn:

CO-1: The statistical distribution of various types of velocities of gas molecules and theories explaining gas behaviors.

CO-2: The various statistical methods used for the studies of properties of gases, liquids and solids.

CO-3: The methods of entropies determination at a given temperature.

CO-4: The various statistical approaches of statistical thermodynamics.

Recommended books:

- R.P.Rastogi, R.R.Mishra, An Introduction to chemical Thermodynamics
- P.W. Atkins, Physical Chemistry,Oxford University press, New York.
- K.L.Kapoor, Advance Physical Chemistry (Vol. 1,2,3,4), MacMillan, India.
- Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar Punjab.

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Course Code: B020907T **Course Credit: 4; 60 hrs.**

Course Title: Magnetisation and Irreversible Thermodynamics

UNIT-I

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

UNIT-II

Orbital and spin moments, Electrons and multielectron systems, Magnetic property of complex compound in relation to their structure, Bohr magneton, L-S and J-J couplings. Electronoic spectra of molecules, Born-Oppenheimer approximation, Franck-Condon principle, Rotational fine structure of Electronic-Vibration transitions, Predissociation spectra, Molecular photoelectron spectroscopy (PES).

UNIT-III

Mossbauer spectroscopy and its principle, Origin of line width, Isomer shift, Quadropole effects, Application of Raman, ESR, NMR and Mossbauer spectra, C^{13} NMR spectroscopy, P^{31} NMR spectroscopy STM (Scanning Tunneling Microscopy)-theory and application, AES (Auger Electron Spectroscopy), EELS (Electron Energy Loss Spectroscopy)

UNIT-IV

Kinetics and mechanism of reactions on surface, Mechanism of surface reactions, Uni and bi-molecular surface reactions, Langmuir-Hinshelwood mechanism, Langmuir-Rideal mechanism, Inhibition of surface reactions, Absolute reaction rate theory of surface reactions.

UNIT- V

Thermodynamic functions for non-equilibrium states, Postulates and methodology, Linear laws, Gibbs equation, Entropy production and entropy flow, Phenamenological equations, Microscopic reversibility and Onsager's reciprocity relations.Transformations of the generalized fluxes and forces, Electrokinetic phenomena, Diffusion, Electric conduction, The stationary non-equilibrium states, States of minimum entropy production.

Course Outcomes: After completing this course, the students will be able to learn:

CO-1: understand various types of magnetic properties, their origin & their temperature dependency.

CO-2: understand principles behind various material characterization techniques such as, Mossbauer spectroscopy, EELS, STM and AES.

CO-3: predicts the number of signals and their positions in C^{13} NMR spectroscopy, P^{31} NMR spectroscopy.

CO-4: understand the spectra obtained in electronic spectroscopy and intensities of lines found in it.

CO-5: Understand the adsorption phenomena on various surfaces and the factors influencing it..

Recommended books:

1. Ebsworth, Rankin, Structural methods in Inorganic Chemistry, ELBS.
2. P.W. Atkins, Physical Chemistry,Oxford University press, New York.
3. R.P.Rastogi, R.R.Mishra, An Introduction to chemical Thermodynamics
4. Colin N. Banwell, Fundamentals of Molecular spectroscopy, McGraw - Hill book company.
5. R.S.Drago, Physical methods in Chemistry, New age publication, New Delhi.
6. K.L.Kapoor, Advance Physical Chemistry (Vol. 1,2,3,4), MacMillan, India.
7. Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar.
8. Keith J.Laidler, Chemical Kinetics, Pearson Education Publisher.
9. Santosh K.Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer.

Course Code: B020908T **Course Credit: 4; 60 hrs.**

Elective Course Title: Environmental Chemistry

UNIT-I

Introduction to Environmental Chemistry: Concept and scope of environmental chemistry, Environmental terminology and nomenclatures, Environmental segments, The natural cycles of environment (Hydrological, Oxygen, Nitrogen)

UNIT-II

Atmosphere: Regions of the atmosphere, Reactions in atmospheric chemistry, Earth's radiation balance, Particles, ion and radicals in atmosphere; Chemistry of ozone layer.

UNIT-III

Hydrosphere: Complexation in natural water and waste-water, Micro-organisms in aquatic chemical reactions, Eutrophication, Microbiology mediated redox reactions.

Lithosphere: Inorganic and organic components in soil, acid-base and ion-exchange reactions in soil, micro and macro nutrients, nitrogen pathways and NPK in soil.

UNIT-IV

Chemical Toxicology: Toxic chemicals in the environments, Impact of toxic chemicals on enzymes. Biochemical effects of arsenic, cadmium, lead, mercury, carbon monoxide, nitrogen oxides, sulphur oxides.

Air Pollution: Particulates, Aerosols, SOx, NOx, COx and hydrocarbon, Photochemical smog. Air-quality standards

UNIT-V

Water Pollution: Water-quality parameters and standards: physical and chemical parameters, Dissolved oxygen, BOD, COD, Total organic carbon, Total nitrogen, Total sulfur, Total phosphorus and Chlorine, Chemical speciation (Pb, As, Hg)

Course Outcomes: After studying this course, the student will be able to understand

CO 1. understand the basic of environment and this will induce and think about pour environment

CO 2. know about different pollution, and way of minimization and measurement technique.

CO 3. understand the basic of toxic material and measurement technique

CO 4. understand the basic of water quality and measurement technique

CO 5. know about different realm form our surrounding

Recommended Books

1. G.W. Vanloon, S.J. Duffer, Environmental Chemistry - A Global Perspective, Oxford University Press (2000).

2. F. W. Fifield and W.P.J. Hairens, Environmental Analytical Chemistry, 2nd Edition (2000), Black Well Science Ltd.

3. Colin Baird, Environmental Chemistry, W.H. Freeman and Company, New York (1995).

4. A.K. De, Environmental Chemistry, 4th Edition (2000), New Age International Private Ltd.,New Delhi.

5. Peter O. Warner, Analysis of Air Pollutants, 1st Edition (1996), John Wiley, New York.

6. S.M. Khopkar, Environmental Pollution Analysis, 1st Edition (1993), Wiley Estern Ltd., New Delhi.

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Course Code: B020909T **Course Credit: 4; 60 hrs.**

Elective Course Title: Analytical Techniques

Unit-I

Thermoanalytical Methods:

a. Thermogravimetry: Apparatus, factors affecting TG, Interpretation of TG curves of $CaC_2O_4.H_2O$ and $MgC_2O_4.2H_2O$

b. Differential Thermal Analysis and Differential Scanning Calorimetry: Apparatus, factors affecting DTA and DSC curves with special reference to heating rate, particle size and packing, measurement of heat of transition, heat of reaction and heat of dehydration of salts and metal hydrates.

Unit-II

Gas Chromatography: Theory, Instrumentation - description of equipment and different parts, columns (packed and capillary columns), detector specifications –thermal conductivity detector, Flame ionization detector, electron capture detector, nitrogen-Phosphorous detector, photo ionization detector, applications in the analysis of gases, petroleum products etc. Hyphenated Analytical Techniques as GC-MS

Unit-III

Atomic absorption and emission spectroscopy: Basic theory, Flame atomization process, flames, nubulization, ionization, droplet prodipitation, mixing, desolvation, interference, lamps, burners, fuels. Nonflame atomization process, general discussion, high temperature furnaces, operating principles, process, interferences, advantages and disadvantages, hydride generation analysis. Flow injection hydride generation. Quartz tube AAS (FI-Hg-QT-AAS). Applications. Origin of spectra, technique, expectation sources, control and multisources, plasma discharge, instrumentation, qualitative analysis, advantages and disadvantages. CpAES, Application (general). Basic principle of inductively coupled plasma atomic emission spectrometry (ICPAES). Applications of AES and ICPAES

Unit-IV

Fundamental and Instrumental aspects of Single crystal X-ray diffraction Technique:

Concepts of crystal structure: Bravais lattice, crystal systems, indexing of lattice planes, translational and rotational symmetry, symmetry elements and their symbols (both numerical and graphical), point group, screw axis, glide plane, HM notation, space groups, centrosymmetric and non-centrosymmetric space groups, space group number and tables (few examples), equivalent position, Braggs law of diffraction, Reciprocal lattice and its relation with direct lattice, Ewald sphere, Different methods of diffraction (Laue, rotating crystal and powder), crystal growth (in brief), crystal mounting techniques using goniometer, centering of crystal, intensity of scattered radiation, structure factor, data collection methods and strategy, data processing, different methods structure solution (direct, Patterson, intrinsic) and refinement, absorption correction, disorder problem, structure validation and publication, intro about CSD database and how to use it. Brief introduction of advanced techniques like Synchrotron X-ray radiation source.

Unit-V

Voltametry: Cyclic voltammetry: Basic principles, three electrode system, reversible, quasireversible, irreversible cyclic voltammograms and application.

Course Outcomes: After studying this course, the student will be able to

CO 1. understand the basic of this course and think & develop new ideas and concepts in analytical chemistry.

CO 2. know about thermoanalytical, chromatographic and spectral techniques.

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CO 3. implement and handle the research and pharmaceutical related instrument and able to interpret the data.

Reference Books:

1. Fundamentals of Analytical Chemistry: D.A. Skoog, D.M. West and F.J. Holler, 1992, 6e
2. Quantitative Inorganic Analysis, A.I. Vogel, 2012, 7e
3. Instrumental Methods of Chemical Analysis: B.K. Sharma, 2011
4. Instrumental Methods of Chemical Analysis: H. Kaur, 2016, 12 e
5. Analytical Chemistry, Gary D. Christian, 2007, 6e
6. Instrumental Methods of Analysis: H.H. Willard, L.L. Merrit, Jr. J.A. Dean, 1974, 5e
7. Hobert H. Willard, D. L. Merrit & J. R. J. A. Dean, Instrumental methods of analysis, C.B.S Publishers and Distributors, 1992.
8. Ewing, Instrumental Methods of Analysis, 1992.
9. Instrumental Methodology of Analysis by Chatwal Anand.

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Course Code: B020910T **Course Credit: 4; 60 hrs.**

Elective Course Title: Computational Chemistry

UNIT: I

Introduction of Internet and Computer, Historical perspectives of computational chemistry Computable quantities like a. Structure b. Potential energy surface c. Chemical properties. Construction of z-matrix a. Diatomic molecules b. Polyatomic molecules

UNIT: II

Force Field/Molecular Mechanics, (i) Common force fields viz., Harmonic and Morse (ii) Existing force fields in popular packages viz., AMBER, CHARMM

UNIT: III

Theory, computation & modelling, Need of approximate methods in quantum mechanics, Computable Quantities – structure, potential energy surfaces and chemical properties, Cost & Efficiency – relative CPU time, software & hardware; Classification of computational methods. Basic principles of Ab initio method - Basics principles of Semiemprical calculations (SE) - Basics principles of Density functional theory (DFT). Ab--Initio and DFT Software Introduction to available software packages viz Gaussian, GAMESS. Orca, NWChem, DALTON d. Graphics Packages - GaussView and Molden.

UNIT: IV

Ab- initio HF calculations: a. Geometry optimization and calculation of HF energy b. Basis sets c. Density function theory (i) Basic theory (ii) Advantage over ab-initio approach (iii) Implementation into popular quantum mechanical package (iv) Applications

UNIT: V

Introduction to QSPR and QSAR, Linear Free Energy Relationships Linear Free Energy Relationships, Molecular discripter, Hansch equation, Application to Real systems a. Biomolecule (i) Methods for modelling Biomolecules (ii) Site-specific interaction (iii) Introduction to computer aided - Drug – design (CADD) b. Synthesis route prediction c. Polymers d. Transition metals

Course Outcomes: After studying this course, the student will be able to

CO-1. Identify and explain the main similarities and difference between theoretical approach such as HF (Hartree-Fock), DFT (Density Functional Theory) and Molecular Mechanics (Force field methods).

CO-2. Describe and identify the various methods advantage/disadvantages for simulating/modelling various scientific problems.

CO-3. Choose and justify suitable methods for calculating electronic properties of simple molecules and crystals and be critically analysing the calculated properties.

CO-4. The program allows graphical input of molecular structure, menu-driven input to quantum chemistry calculational programs, and graphical analysis of molecular properties.

CO-5. Useful in analyzing theproperties of short-lived transition states and intermediates and species that are difficult to handle inside a laboratory such as explosives.

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CO-6. Computational methods can be used to compute the properties of unknown moleculesand will be helpful in testing the properties of molecules in-silico before actualexperiment has been carried out.

Books Suggested

1. Modern quantum Chemistry, N.s. Ostlund and A. Szabo, McGraw Hill.
2. Methods of Molecular Quantum Mechanics R. McWeeny and B.T. Sutclifffe. Academic Press.
3. Density Functional Theory :' Atoms and Molecules R.G. Parr and W. Yang. Oxford
4. Explorng Chemistry with Electron Structure Methods.
5. Foresman and E. Frish. Gaussian Inc.
6. Semi-empirical MO theory. J. Pople and D.L. Beveridge.

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Course Code: B0209111P **Course Credit: 4; 120 hrs.**

Lab Course Title: Inorganic Chemistry Practical-I

1. **Separation of a mixture of cations/anions by paper chromatographic technique using aqueous/non-aqueous media:**

a. Pb^{2+} and Ag^{+} (aqueous and non-aqueous media)
b. Co^{2+} and Cu^{2+} (non aqueous media)
c. Cl^{-} and I^{-} (aqueous – acetone media)
d. Br^{-} and I^{-} (aqueous – acetone media)

2. **Ion-exchange Method of Separation**

a. Separation of Zn^{2+} and Mg^{2+} on an anion exchanger
b. Separation of Co^{2+} and Ni^{2+} on an anion exchanger

Course Code: B020912P **Course Credit: 4; 120 hrs.**

Lab Course Title: Organic Chemistry Practical-I

A. Separation and identification of organic compounds using chemical methods from organic mixtures containing up to three components

B. Preparations of Organic compounds involving two and three stages:
Typical preparations from which the two and three stage preparations can be chosen are:
1. Toluene — p-nitrotoluene — p-nitrobenzoic acid — p-amino benzoic acid
2. Hydroquinone — Benzoquinone — 5- Hydroxy benzoxathiole-2-one —5-Acetoxy benzoxathiol-2-one
3. Benzene — Acetopheneone — Acetophenone oxime — Acetanilide
4. Benzaldehyde — Benzoin — Benzil — Benzillic acid
5. Acetylacetone — 4,6-dimethylpyridine-2-mercaptopyrimidine — 4,6-dimethyl-2-hydrazinpyrimidine — 1-(4'-6'-dimethylpyridine-2'yl) 3,5-dimethylpyrazole
6. Nitrobenzene — m-dinitrobenzene — m-nitroaniline — m-nitrophenol
7. Phthalic acid — phthalic anhydride – phthalimide — Anthranilic acid
8. Acetophenone — Benzalacetophenone — epoxide
9. Cyclohexanone —Cyclohexanone oxime—caprolactam
10. Phthalic anhydride—o-benzolylbenzoic acid—anthraquinone.

C. Verification of Lambert Beer's Law using broriocresol green reagent.
D. Estimation of carbohydrates, protein, aminoacids, ascorbic acid, blood cholesterol and aspirin in APC tablets by UV-visible Spectrophotometric method.

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Course Code: B02091P **Course Credit: 4; 120 hrs.**

Lab Course Title: Physical Chemistry Practical-I

1. Kinetics of Pd(II) catalysed oxidation of reducing sugars by N-bromoacetamide in acidic medium.
2. Conductometric titration of mixtures of acid and base.
3. Determination of freezing point depression constant.
4. Determination of specific and molecular rotation of sucrose in different conc. and to determine the conc. of given solution.
5. Determination of distribution coefficient of
   - Acetic acid between water and benzene by partition method
   - Benzoic acid between water and benzene by partition method
6. Test the validity of Beer-Lambert's law and determination of the conc. of glucose solution with the help of colorimeter.

Course Code: B020914R **Course Credit: 4; 120 hrs.**

Course Title: Experiment, Result & Discussion

The allotted research topic in the VIIIth semester will be continued in the IXth semester. Student will perform experiment/calculations and he/she will collect the data. The collected data will be summarised and prepare the dissertation. At the end of the semester, students have to submit a dissertation and present their findings and progress of the allotted research work.

SEMESTER X

Course Code: B021001T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Coordination Polymers, Cages, Clusters and Nanostructures

UNIT-I

Coordination Polymers
Classification, types of metal-organic frameworks (MOFs), Synthetic strategies, characterization, properties and applications.

UNIT-II

Metal Carbonyls and related Compounds
Preparation structure and properties; bonding in metal carbonyls, variants of CO bridging vibrational spectra of metal carbonyls, principle reaction types of metal carbonyls, metal nitrosyl.

UNIT-III

Polyhedral Boranes
Higher boranes, carboranes, metallo-boranes and metallo-carboranes – Structure and bonding in the light of Wade's and Jemmis' Rules.

UNIT-IV

Nanoscience
Introduction to Nanoscience, unique properties of nanomaterials, classifications of nanomaterial. Band gaps, exciton, quantum confinement. General methods of synthesis of nanomaterials and nanostructures: top down, bottom up approach. Characterizations techniques of nanomaterials. Applications of nanomaterials.

UNIT-V

Alkoxides Properties; structural aspects of various types of alkoxides – Industrial applications and catalytic aspects of metal alkoxides.

Course outcomes (COs): After completing the course, students will be able to:
CO-1: Corelate structure of a metal compound and its magnetic properties.
CO-2: Design a complex with required magnetic properties.
CO-3: Explore more about complexes like boranes, carboranes, metal carbonyles etc and their applications.
CO-4: Insights and behaviour of metal clusters

Recommended Books

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harper & Row.
3. Inorganic Electronic Spectroscopy, A.B.P. Lever, Elsevier.
4. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
5. Introduction to Ligand fields; B.N. Figgis, Wiley, New York.
6. Modern Aspects of Inorganic Chemistry; H.J. Emeleus and Sharpe.
7. Introduction to Ligand Field Theory; C. J. Ballahyen, McGraw Hill, New York.
8. Organometallic Chemistry; R.C.Mehrotra and A.Singh, New Age International.
9. Concepts and Models of Inorganic Chemistry; B. Douglas, D.H.McDaniel and J.J.Alexander; John Wiley.
10. The Organometallic Chemistry of the Transit ion Metals; R.H. Crabtree, John Wiley.

SUGGESTED WEB SOURCES:
1. https://nptel.ac.in/course.html

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Course Code: B021002T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Main group and inner-transition elements

Unit-I

Alkali and alkaline earth metals
Preparation, Structure, Bonding and Applications of polyether complexes of alkali and alkaline earth metals

Unit-II

p-block elements: Classification, synthesis and structure of carbides, silicates and polyphasphazenes

Unit-III

Inner Transition Elements I: Comparison of characteristics of inner transition and transition metals, variable oxidation state, separation technique. Magnetic properties and absorption spectra.

Unit-IV

Inner Transition Elements II: Spectral and magnetic properties, redox chemistry, analytical applications of lanthanides and actinides.

Unit-V

Magnetic Properties: Magnetic behaviours, recent methods of magnetic susceptibility measurements, anomalous magnetic properties of transition metal complexes, spin crossover phenomena, magnetic properties of binuclear metal complexes involving metal-metal exchange interaction (Bleaney-Bower equation).

Course outcomes (COs): After completing the course, students will be able to:
CO-1: Undrestand symmetry, group theory, and Stereochemistry
CO-2: Undrestand Metal-Ligand Equilibria in solution
CO-3: undestand the bonding concepts involved in Coordination compounds
CO-4: utilize this knowledge for complex formation of research interest.

Recommended Books

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harper & Row.
3. Chemical Applications of Group Theory; F.A. Cotton, Wiley, New York.
4. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
5. The Chemical bond; J.N.Murre l, SFA Kettle and JM. Tedder; Wiley, New York.
6. Modern Aspects of Inorganic Chemistry; H.J. Emeleus and Sharpe.
7. Concepts and Models of Inorganic Chemistry; B. Douglas, D.H. McDanie l and. J.J.Alexander; John Wiley and Sons.
8. Inorganic Chemistry, A Modern Introduction; T Moeller, John Wiley and Sons.

SUGGESTED WEB SOURCES:
1. https://nptel.ac.in/course.html
2. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5
3. https://swayam.gov.in/explorer?category=Chemistry

Course Code: B021003T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Solid State and Nuclear Chemistry

UNIT-I

Solid – State Chemistry I

Theory of metals free electron, valence bond and molecular orbital theories, conductors, insulators and Semiconductors. Superconductivity.

UNIT-II

Solid – State Chemistry II

Alloys and intermetallic compounds. Hume-Rothery Lattice defects in ionic crystals – stoichiometric and non-stoichiometric defects.

UNIT-III

Nuclear fission and fusion

Nuclear fission and fusion reactions, energy release in fission chain reactions and fusion reaction, controlled release of fission energy use of moderators;

UNIT-IV

Nuclear reactors including breeder reactors, principle of atom and hydrogen bombs, nuclear Fuels-Fuel cycle & Fuel reprocessing.

UNIT- V

Radiochemical Analysis

Activation analysis, Radiometric and radio – release methods, Activation Analysis Tracer Techniques and Dilution Analysis, Radiometric titrations.

Course outcomes (COs): After completing the course, students will be able to:

CO-1: Explain different types of chemical reactions of inorganic chemistry.
CO-2: Explain photochemical reactions.
CO-3: Solve problems related to nuclear chemistry
CO-4: Propose new synthetic routes for the compounds

Recommended Books

1. Mechanism of Inorganic Reactions; F.Basolo and R.G. Pearson, John Wiley and Sons, New York.
2. Inorganic Reaction Mechanism; M.L. Tobe; Nelson, Wlaton and Thames
3. Inorganic Chemistry; K.F. Purcell, J.C. Kotz; Holt-Sanders International Editions; Philadelphia.
4. The Chemistry of Molten Salts; H. Bloom Benjamin, New York.
5. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Finke, University Science Books.
6. The Organometallic Chemistry of the Transition Metals; R.H. Crabtree, John Wiley.
7. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International
8. Coordination Chemistry; Banerjea; Tata McGraw Hill.
9. Inorganic Chemistry, A Modern Introduction; T. Moeller; John Wiley and Sons.
10. Concepts and Models of Inorganic Chemistry; B. Douglas, D.H. McDaniel and J.J. Alexander; John Wiley and Sons Inc.
11. Essentials of Nuclear Chemistry – H. J. Arnikar.
12. Radio Chemistry & Nuclear Chemistry – G.Choppin, J.O. Liljenzin & J.Rydberg.

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Course Code: B021004T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Chemistry of Natural Products

UNIT- I

Bio-synthesis of Natural Products

a. The acetate hypothesis, poly β-Ketoacids, Biosynthesis, Biogenesis Primary and Secondary reactions involved in biosynthesis.
b. Isoprene rule, mevalonic acid from acetyl Co-enzyme A. Biosynthesis of mono, sesqui,di and triterpenes.
c. Shikimic acid pathway for biosynthesis of aromatic ring.
d. General biosynthesis of alkaloids.

UNIT- II

Terpenoids and Carotenoids: Classification, isoprene rule. Structure determination, stereochemistry, synthesis of the following representative molecules: Citral, α-terpenol, Farnesol, Santonin, Abietic acid and β-carotene, Menthol. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

UNIT- III

Alkaloids: General methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, Structure, stereochemistry and synthesis of the following : Ephedrine, Nicotine, Quinine and Morphine. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

UNIT- IV

Steroids: Basic skeleton Diel'shyadrocarbon and stereochemistry, structure determination and synthesis of Cholesterol, Bile acid, Androsterone. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

UNIT- V

Plant Pigments: General methods of structure determination, synthesis of Apigenin, Quercetin Cyanidin Hirsutidine, Quercetin-3-glucoside. For structure elucidation emphasis is to be placed on the use of spectral data wherever possible.

Course outcomes (COs): After completing the course, students will be able to:

CO-1. Classification, biosynthesis, stereochemistry and synthesis of some important terpenoids and carotenoids.
CO-2. Nomenclature, structure elucidation, physiological action and synthesis of Alkaloids.
CO-3. Occurence, basic structure, Isolation and synthesis of some prominent Steroids.
CO-4. Types of carbohydrates, structure elucidation, biological importance and Blood sugar.
CO-5. Types of plant pigments, their structure determination, isolation and synthesis of some significant plant pigments.

Recommended Books:

1. Designing Organic Synthesis, S.Warren, Wiley.
2. Organic Chemistry, Vol. 2, I.L. Finar, ELBS.
3. Heterocylic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
4. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergaman Press.
5. Natural Products: Chemistry and Biology Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.

Course Code: B021005T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Carbohydrates and Vitamins

UNIT- I

Carbohydrates

Structure (excluding conformational analysis) and biological functions of monosaccharides (glucose, fructose and galactose) and their derivatives like glycosides, deoxy sugars, myoinositol. Disaccharides- sucrose, lactose and maltose. Structure and biological functions of Structural polysaccharides (cellulose and chitin) and Storage polysaccharides (starch and glycogen) Heteropolysaccharides-Glucosaminoglycans / mucopolysaccharides.

UNIT- II

Vitamins: Structure determination including synthesis of Thiamine (Vitamin B1), Biotin (Vitmin H) and Vitamin E

UNIT- III

Disconnection Approach-I

An introduction of synthons and synthetic equivalents, general principles of the disconnection approach, functional group interconversions, the importance of order of events in organic synthesis, one group C-X and two group C-X disconnections, one group C-C disconnection, chemoselectivity, regioselectivity, regiospecificity, stereoselectivity and stereospecificity, reversal of polarity.

UNIT IV

Disconnection Approach-II

Principle of protection of alcoholic, amino, carbonyl and carboxylic groups. Two group C-C disconnection- Diels Alder reactions, 1,3-difunctionalized compounds and □,□ unsaturated carbonyl compounds, control in carbonyl condensations, 1,5-difunctionalized compounds-Michael addition and Robinson Annelation. Disconnection approach towards the synthesis of juvabione and cortinsone.

UNIT V

Protecting Groups: Principle of protection of alcoholic, amino, carbonyl and carboxylic groups.

Course Outcomes: After the completion of this course, the learner will be able to

CO1: understand the general aspects of carbohydrate and its natural product including structures, stereochemistry and synthesis.

CO2: be acquainted with mechanistic details of the methods of preparation and reactions of heterocyclic compounds.

CO3: familiar with basic concepts of disconnection approach, one & two-group C-X and C-C disconnections, chemoselectivity, reversal of polarity, amine synthesis, stereoselectivity, stereospecificity, regioselectivity and regiospecificity.

CO4: apprise of protection of important functional groups viz. alcoholic, amino, carbonyl and carboxylic groups and to apply the concept of disconnection approach for the synthesis of drug molecules.

Recommended books:

1. Designing Organic Synthesis, S.Warren, Wiley.
2. Organic Chemistry, Vol. 2, I.L. Finar, ELBS.
3. Heterocylic Chemistry, T.L. Gilchrist, Longman Scientific Technical.
4. Comprehensive Heterocyclic Chemistry, A.R. Katritzky and C.W. Rees, eds. Pergaman Press.
5. Natural Products: Chemistry and Biology Significance, J. Mann, R. S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.

Course Code: B021006T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Biomolecules

UNIT- I

Enzymes: Introduction and historical perspective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature, classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling. Enzyme kinetics, Michaelis Menten and Lineweaver-Burk plots, reversible and irreversible inhibition. Mechanism of Enzyme Action: Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion.

Biotechnological Applications of Enzymes Large-scale production and purification of enzymes, techniques and methods of immobilization of enzymes, effect of immobilization on enzyme activity, application of immobilized enzymes, enzymes as targets for drug design. Clinical uses of enzymes, enzyme therapy, enzymes and recombinant DNA technology.

UNIT- II

Nucleic Acids: Retro-synthetic analysis of Nucleic Acids - Nucleotides, Nucleosides, Nucleobases (A, T, G, C and U), Sugars (Ribose and deoxyribose). Assembly of oligonucleotide chain: Synthesis of polymer support, Nucleosides and Nucleotides, solid phase synthesis of oligo-nucleotides (DNA/RNA) through phosphoramidite and phosphorothionate approach. Application of protecting groups (-NH_2 and –OH functions) and their deprotection and purification.

UNIT- III

Lipids: Fatty acids, essential fatty acids, structure and function of triacylglycerols, glycerophospholipids, sphingolipids, cholesterol, bile acids, prostaglandins. Lipoproteins - composition and function, role in atherosclerosis. Lipid metabolism - β-oxidation of fatty acids

Protiens: Primary, secondary, tertiary and quaternary structures, enzymes, active sites, allosteric sites and mechanism of their action, e.g. Chymotrypsin

UNIT- IV

Antibiotics: Cell wall biosysnthesis and protein synthesis inhibitors: Penicillins and semi-synthetic penicillins. Medicinal uses of penicillin G, β-lactamase and narrow spectrum of activity (structure elucidation and synthesis excluded). Introduction and discovery of cephalosporins (structure elucidation and synthesis excluded).

UNIT- V

Pyrethroids, Rotenones and Pheromones: Occurrence, classification, Biogenesis and physiological effects. Natural and synthetic pyrethroids, Rotenones and pheromones. Synthesis of bombykol.

COURSE OUTCOMES: After the completion of this course, the learner will be able to:

CO1: Understand the basics of enzymes (classification and nomenclature) and their role in biological systems.

CO2: Know the basics of antibiotics mainly focusing to the penicillin.

CO3: identify various classes of biomacromolecules and their building blocks

CO4: understand the flow of information from genetic material to proteins and other biomolecules

CO5: Understand mode of action of pyrethroids, rotenones, pheromones and its synthesis and development.

Books Suggested:

1. Organic Chemistry, Vol 2, I. L. Finar, ELBS.
2. Natural Products: Chemistry and Biology Significance, J.Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.
3. Biochemistry, A.L. Lehninger.
4. Outlines of Biochemistry, Cohn & Stumpf.

5. Wilson and Gisvold's Text book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Dorge.
6. Burger's Medicinal Chemistry and Drug Discovery Vol-I Ed. M.E. Wolf, John Wiley.
7. Goodman and Gilman's Pharmacological Basis of Therapeutics, McGraw - Hill.
8. Natural Product Chemistry, Jagdamba Singh, Syed M. Ali, Jaya Singh
9. Bioorganic, Bioinorganic and Supramolecular Chemistry, P.S. Kalsi, New Age International (P) Limited

Suggested Web Sources:

1. https://nptel.ac.in/course.html
2. https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=5
3. https://swayam.gov.in/explorer?category=Chemistry

Course Code: B021007T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Solution and Advanced Quantum Chemistry

UNIT- I

Ideal and non-ideal solutions, Inter-connection between Raoult's law and Henry's Law, Determination of Partial Molar Properties, Thermodynamic functions of mixing of non-ideal solutions, Excess thermodynamic functions.Gibbs-Dohme-Margules equation and its applications, Activity and activity coefficients, Activity coefficients from excess thermodynamic functions, The theory of Van Laar, Scatchard Hildebrand theory, Wilson model and Flory-Huggins theory.

UNIT- II

Concept of operators in quantum mechanics—operators for velocity, kinetic energy, momentum and angular momentum, Derivation of Heisenberg's uncertainty principle, Solution for Hydrogen atom, Born-Oppenheimer approximation, Valence bond theory and its application to homonuclear (Hydrogen) and heteronuclear (HCl) diatomics, LCAO-MO treatment of hydrogen molecule ion. Comparative study of MO and VB theory.

UNIT-III

Huckel molecular orbital theory and its application to hybridization systems (ethylene, butadiene, allyls and benzene), Calculation of delocalization energy, Physical significance of charge density and bond order, Calculation of bond length, Pauling and Wheland's modification in HMO theory and it application to heteromolecules (pyrimidine), Perturbation methods in LCAO-MO theory, Extended Huckel molecular orbital theory and SCF-MO method.

UNIT-IV

Comparison of homogeneous and heterogenous reactions, Study of equilibrium constant and steady state treatment for Arrhenius and Vant Hoff's complexes, Influence of substituents on reaction rates (inductive and electromeric effects), Linear free energy relationship, Taft equation, compensation effect, Hemmett acidity tunetions.

UNIT-V

Mechanism of electrode reactions, Over potential, The current-potential relation, The Tafel equation, Hydrogen overvoltage and decomposition potential, Butler-Volmer equation, H_2-Evolution mechanism.

Course Outcomes: After completing this course, the students will be able to learn:

CO-1. The various properties of solutions, its related laws and theories.
CO-2. The different operators, Heisenberg's uncertainty principle.
CO-3. The various bonding theories, their characteristics and limitations.
CO-4. Huckel molecular orbital theory and Perturbation methods in LCAO-MOtheory.
CO-5. Steady state treatment for Arrhenius and Vant Hoff's complexes and Influence of substituents on reaction rates
CO-6. The kinetics of different types of reactions and factors which depends on it.
CO-7. The electrode reactions and consequences of electrode reactions.

Recommended books:

1. S.Glasstone, An introduction to Electrochemistry, D. Van Nostrand company Inc..
2. K.L.Kapoor, Advance Physical Chemistry (Vol. 1,2,3,4), MacMillan, India.
3. I.N. Levine, Quantum Chemistry.
4. Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar Punjab.
5. Keith J.Laidler, Chemical Kinetics, Pearson Education Publisher.
6. Santosh K.Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer.

7. V.K.Thankappan, Quantum Mechanics through Problems, New Age International Publishers, New Delhi.
8. K.K.Rohatgi- Mukherjee, Fundamentals of Photochemistry,New Age International Publishers, New Delhi.
9. R.K.Prasad, Quantum Chemistry, New Age International Publishers, New Delhi.
10. R.P.Rastogi, R.R.Mishra, An Introduction to chemical Thermodynamics
11. Colin N. Banwell, Fundamentals of Molecular spectroscopy, McGraw - Hill book company.
12. R.S.Drago, Physical methods in Chemistry, New age publication, New Delhi.
13. K.L.Kapoor, Advance Physical Chemistry (Vol. 1,2,3,4), MacMillan, India.
14. Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar Punjab.
15. Keith J.Laidler, Chemical Kinetics, Pearson Education Publisher.
16. Santosh K.Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer.

Course Code: B021008T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Solid Advance Electro Chemistry

UNIT- I

Classification of solids, Bonding in solids, covalent, metallic, ionic and molecular crystals, Lattice energy of crystals, Cohesive energy, Conduction in solids and super conductance, Electronic structures of solids, Free electron theory, Fermi-gas theory and band theory of solids, Metals, semi-conductors and insulators, Intrinsic extrinsic p-type and n-type semi-conductors.

UNIT- II

Vapour pressure, compressibility viscosity and sound velocity, Internal pressure and its determination, Significance of internal pressure, solubility parameter and cohesive-energy-density, Free volume of liquids and its determination, Application of free volume and its relation with energy and heat of vaporization.

UNIT- III

Partition function of a liquid, Equation of state in terms of partition function, Outline of the theory of liquid state:JSimple cell theory (Eyring equation) and cell model theory of Lennard-Jones and Devonshire, Eyring's free volume theory of liquid viscosity, Effect of pressure on viscosity,
Thermodynamic functions of ideal and non-ideal liquid mixtures, Partial molar properties of liquid mixtures, Determination of partial molar volume and partial molar enthalpy,

UNIT- IV

The triumph and limitations of Debye-Huckel theory of activity coefficients, Electrical potential and mean activity coefficient in the case of ionic clouds with finite sized ions, The ion size parameter and comparison of the finite-ion-size model with experiment,Asymmetry and electriphoretic effects, Stoke's law and Walden product, Debye-Huckel-Onsager equation, Conductance ratio and the Onsager slope, Verification of Debye-Huckel-Onsager equation, Conductivity of weak electrolytes and conductance in nonaqueous solvents. Modifications of Debye-Huckel-Onsager equation,Fuoss-Onsager and other equations, Wien and Debye-Fakenhagen effects.

UNIT- V

Viscosity of electrolyte solutions-Jones-Dole equation and significance of A and B coefficients, Ion association in an electrolyte solution, Formation of pairs, triplets etc, The probability of finding oppositely charged ions near each other, Bjerrum theory of ion association.

Course Outcomes: After completing this course, the students will be able to learn:

CO-1. The properties of various kinds of solids and theoretical explanation.

CO-2. The various properties of liquids and their related phenomena.

CO-3. The methods to determine the liquid's properties.

CO-4. The factors affecting the movement of ions in electrolyte solution and their theoretical basis.

CO-5. The different types of interactions of ions taking place in an electrolytic solution.

Recommended books:

1. A.R.West, Solid state chemistry and its application, Plenum.
2. D.K.Chakrabarty, Solid state chemistry, New Age International Publisher.
3. S.Glasstone, An introduction to Electrochemistry, D. Van Nostrand company Inc..
4. K.L.Kapoor, Advance Physical Chemistry (Vol. 1,2,3,4), MacMillan, India.
5. Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar Punjab.
6. Santosh K.Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer.
7. R.P.Rastogi, R.R.Mishra, An Introduction to chemical Thermodynamics.
8. S.Glasstone, An introduction to Electrochemistry, D. Van Nostrand company Inc..
9. Puri Sharma Pathania Kalia, Advanced physical Chemistry, Vishal Publication, Jalandhar Punjab.
10. Keith J.Laidler, Chemical Kinetics, Pearson Education Publisher.
11. Santosh K.Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer.

Course Code: B021009T **Course Credit: 4; 60 hrs.**

Specialization Course Title: Polymer Chemistry

UNIT–I

Polymer Characterisation **12 Hrs**

Polymerisation process and mechanism: condensation, addition, radical, chain, ionic and coordination and co–polymerisation. Kinetic of initiation retardation, chain polymerization and ionic polymerization (anionic and cationic), Copolymerisation (with special reference to monomer reactivities ratios). Coordination polymerization, Degradation of polymers (oxidative, chemical and photolytic), Polyelectrolytes.

UNIT–II

Structure and Properties **12 Hrs**

Morphology and order in crystalline polymers–configurations of polymer chains. Crystal structure of polymers. Morphology of crystalline polymers, strain induced morphology, crystallisation and melting. Polymer structure and physical properties– crystalline melting point Tm, melting points of homogeneous series, effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g–relationship between Tm and T_g, effects of molecular weights, diluents, chemical structure, chain topology, branching and cross linking. Property requirements and polymer utilisation.

UNIT–III

Polymer Processing **12 Hrs**

Plastics, elastomers and fibers. Compounding. Processing techniques–calendaring, dye casting, rotational casting, film casting, injection moulding, blow moulding, extrusion moulding, thermoforming, reinforcing and fibre spinning. Analysis and testing of polymers– chemical analysis of polymers, spectroscopic methods, microscopy, thermal analysis and physical testing–strength, fatigue, impact. Tear resistance hardness and abrasion resistance.

UNIT–IV

Biopolymers And Biodegradable Polymers **12 Hrs**

Biopolymers, applications and use, common biopolymers such as collagen, gelatin, starch, silk fibroin.Types of biodegradable polymers, bio based polymers, Starch based polymers, Cellulose based polymers, Chitin and Chitosan,carrageenan, alginate, cellulose, xanthan gum, guar gum, dextron, Gellan gum. Bacterial Polyesters, Synthetic Biodegradable Polymers, Polymers from BioBased Monomers.

UNIT–V

Applications Of Commercial Polymers **12 Hrs**

Polyethylene, PVC, Polyamides, Polyesters, Phenolic resins, Epoxiresins, Silicone polymers. Functional polymers–Fire retarding polymers and electrically conduction polymers. Biomedical polymers–contact lenses, dental polymers, artificial heart, kidney, skin and blood cells

Course Outcomes: After completing this course, the students will be able to:

CO-1. Define various terms used in polymer chemistry.
CO-2. Learn the mechanism of polymerization.
CO-3. Classify the polymers on the basis of forces, properties, and mechanism of polymerization.
CO-4. Learn the various applications of synthesized polymers and their properties.
CO-5. Learn the methods of analysis of polymers.
CO-6. Learn the synthesis of various polymers and conditioned to tailoring the properties of them.

Reference Book

1. F.W. Billmeyer, Text Book of Polymer Science, Wiley–Interscience, New York.1971.

2. V.R. Gowariker, N.V. Viswanathan & J. Sreedhar, Polymer Science, John Wiley & Sons, New York, 1986.
3. K. Takemoto, Y. Inaki& R.M. Ottanbrite, M. Kamachi, Functional Monomers &Polymers, CRC Press, 1997.
4. H.R. Alcock& F.W. Lambe, Contemporary Polymer Chemistry, PrenticeHall, USA.
5. J.M.G. Cowie, Physics & Chemistry of Polymers, Blacke Academic Press, 1993.
6. Handbook of Biodegradable Polymers :CatiaBastioli
7. Biopolymers and biomaterials:Padinjakkara, Aneesa Souza, Fernando Gomes Thankappan,

Course Code: B021010T **Course Credit: 4; 60 hrs.**

Elective Course Title: Reagents and Reactions

UNIT: I

Regents in Organic Synthesis I: Use of following reagents in organic synthesis and functional group transformation (including stereochemistry where possible) Complex metal hydrides – $NaBH_4$, $LiAlH_4$, DIBAL, diborane, diisoamylborne, thexylborane, 9-BBN, isopinocamphenyl and diisopino-campherylborame, catechoborane; Gilman's reagent; Lithium disopropyl amide (LDA)

UNIT: II

Regents in Organic Synthesis II: Use of following reagents in organic synthesis and functional group transformation (including stereochemistry where possible): Dicyclohexylcarbcarbodimide (DCC); 1, 3-Dithiane (Reactivity Umpolung); Trimethylsily iodide; Tri n-butyltin hydride; DEAD

UNIT: III

Regents in Organic Synthesis III: Use of following regents in organic synthesis and function group transformation (including stereochemistry where possible) : DDQ; Hydrazine and phenylhydrazine; Nucleophilic heterocyclic carbenes (NHC); Nitrogen, Sulphur and Phosphorus Ylide: Preparation and their synthetic applications.

UNIT: IV

Name reactions: Selective Organic name reaction and their Synthetic Application Stork Enamine reaction; Ene Reaction; Barton Reaction; Hofmann-Loffler-Freytag Reaction; Shapiro Reaction Baylis-Hillman Reaction, Stetter Reaction.

UNIT: V

Application of Pd(0) and Pd(II) complexes in organic synthesis: Stille, Suzuki and Sonogashira coupling, Heck reaction and Negishi coupling.

Course Outcomes: After completing this course, the students will be able to:

CO-1: regents for organic synthesis and their mechanism
CO-2: regents for complex organic synthesis and their mechanism
CO-3: addition reactions between carbon- carbon multiple bonds and hetero atom and carbon multiple bonds and mechanism of some specific name reactions.
CO-4: elimination reactions with the help of specific examples of elimination reactions.
CO-5: organometallic reagent for different organic synthesis

Recommended Books

1. Organic Chemistry, J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford Press.)
2. Advanced Organic Chemistry, A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
3. Advanced Organic Chemistry, J. March, 6th Ed.
5. Advance Organic synthsis, Jagdamba Singh and L. D. S. Yadav, Pragati Publication

Course Code: B021011T **Course Credit: 4; 60 hrs.**

Course Title: Elective II: Supramolecular Chemistry

UNIT-I

Definition, Development and Classification, Binding Constants, Supramolecular interactions, Ionophores, Porphyrin and other Tetrapyrrolic Macrocycles, Coenzymes, Neurotransmitters, DNA and Biochemical Self-assembly

UNIT-II

Podand, Crown Ether, Cryptand, Spherand - Nomenclature, Selectivity and Solution Behaviour. Alkalides, Electrides, Calixarenes, Siderophores

UNIT-III

Challenges and Concepts, Biological Receptors, Conversion of Cation Hosts to Anion Hosts, Neutral Receptors, Metal-Containing Receptors, Cholapods

UNIT-IV

Contact Ion Pairs, Cascade Complexes, Remote Anion and Cation Binding Sites, Symport and Metals Extraction

UNIT-V

Clathrates, Inclusion Compounds, Zeolites, Intercalates, Coordination Polymers, Guest Binding by Cavitands and Cyclodextrins, Concepts, Crystal Nucleation and Growth, Understanding Crystal Structures, Polymorphism, Cocrystals

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

CO-1: provide insight into the various supramolecular interactions

CO-2: appreciate the basis of supramolecular chemistry in terms of examples from nature

CO-3: understand and analyze the structure-function correlations from supramolecular Perspective

CO-4: apply basic concepts of analytical and spectroscopic methods to understand host-guestchemistry

CO-5: apply Self-assembly and crystal engineering approach to understand host-guest chemistry

Recommended Books

1. J. W. Steed & J. L. Atwood (2009), Supramolecular Chemistry, 2nd Edition, John Wiley
2. G.R. Desiraju (1989), Crystal Engineering. The Design of Organic Solids, Elsevier
3. G. R. Desiraju, J. J. Vittal, A. Ramanan (1989), Crystal Engineering -A Textbook, World Scientific-IISc Press
4. Recent papers from journals and reviews and monographs, etc

Course Code: B021012T **Course Credit: 4; 60 hrs.**

Course Title:–Elective II: Medicinal & Pharmaceutical Chemistry

UNIT-I

Drug Targets Introduction to medicinal chemistry intermolecular binding forces, Introduction to various drug targets; Proteins- primary, secondary and tertiary structure, protein function, proteomics; Enzymes- catalytic role, active site, allosteric binding, feedback control, binding interactions, isozymes, co-factors; Receptors- types of receptors, their roles, neurotransmitters, hormones, receptor activation and regulation, signal transduction; Nucleic acids- DNA, primary and secondary structure of DNA, function for DNA molecular biology and genetic engineering.

UNIT-II

Drug-target binding Introduction to Pharmacodynamics and pharmacokinetics, Enzymes as drug targets- types of enzyme inhibitors, medicinal use of enzyme inhibitors with examples; Receptors as drug targets- agonists, antagonists, allosteric modulators, partial agonists, inverse agonists, desensitization, tolerance and dependence, affinity and efficacy; Nucleic acids as drug targets- Intercalating agents, topoisomersae poisons, alkylating/metallating agents, chain cutters, chain terminators, examples of medicinal use. Miscellaneous drug targets

UNIT - III

Drug discovery, design and development Development of new drugs, concept of lead compounds and lead modifications, bioassays, in vitro, in vivo and in silico tests, HTS, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism. Theories of drug activity, Quantitative structure activity relationship, Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric factors, toxicity studies, clinical trials, regulatory process of getting drugs into markets.

UNIT - IV

Types of Medicinal Agents Antibacterial agents-history, bacterial cell, classification of antibacterial agents, examples; Antiviral agents- introduction to viruses, life cycle, vaccination, classification of antiviral drugs; Anticancer agents- Introduction to cancer and cancer treatment, classification of anticancer drugs; Cardiovascular drugs, Psychoactive drugs, Synthesis of the following drugs- ciprofloxacin and cisplatin.

UNIT – V

Drug Synthesis: Anxiolytics: Benzodiazepines; Neuroleptics: Phenothiazines; Hypnotics and Sedatives: Piperidinediones; Local anesthetics: Aminobenzoic acid and its derivatives; Anti: coagulants – 1,3 – Indanedione derivatives; Hypoglycemic agents: Sulfonylureas; Antihistaminic agents: Ethylenediamine derivatives; Antimalarials: Aminoquinolines; Analgesics and Antipyretics :Paracetamol, Phenylbutazone; Anti-inflammatory: Diclofenac

Course Outcomes: After completing this course, the students will be able to:

CO-1. the structural activity relationship of different class of drugs.

CO-2. the synthesis of drug molecules using the reactions of synthetic organic chemistry.

CO-3. well acquainted with the synthesis of some important class of drugs.

CO-4. the mechanism pathways of certain class of medicinal compounds and their modes of action with receptors.

CO-5. the chemistry of drugs with respect to their pharmacological activity

Recommended Books:

1. Thomas L. Lemke, David A. Williams, Victoria F. Roche, S. William Zito, Foye's

Course Code: B021013T **Course Credit: 4; 120 hrs.**

Lab Course Code: Inorganic Chemistry Practical-II

1. Iron – phenanthroline complex: Job's method.
2. Zirconium – Alizarin Red-S complexes: Mole-ratio method.
3. Copper-Ethylene diamine complexes: Slope-ratio method.
4. Iron-thiocyanate complex-Ionophoretic method

Course Code: B021014T **Course Credit: 4; 120 hrs.**

Lab Course Code: Organic Chemistry Practical-II

1. Estimation of $-NO_2$ group in organic compounds.
2. Isolation of casein from milk, piperine from black papper and nicotine from tobacco.
3. Applications of NMR spectrocopy (^1H &^{13}C), UV, IR and Mass Spectroscopy in structure determination of organic and biologically important compounds

Course Code: B021015T **Course Credit: 4; 120 hrs.**

Lab Course Code: Physical Chemistry Practical-II

1. Kinetics of Ir(III) catalysed oxidation of reducing sugars by sodium periodate in alkaline medium.
2. Kinetics of Ru(III) catalysed oxidation of organic substrates by Ce(IV) sulphate in acidic medium
3.Determination of rate constant of inversion of sugar (cane sugar) by acid using Polarimeter.
4.To find the specific rotation of sugar solution by using a polarimeter.
5. Preparation of the colloidal solution of As_2S_3 sol and $Fe(OH)_3$ sol.
6. Determination of the phosphate conc. in a soft drink colorimetrically.

Course Code: B021016R **Course Credit: 4; 120 hrs.**

Research Course Code: Research Project Report /Thesis

The allotted research topic in the VIIIth semester will be continued in the Xth semester. During Xth semester, student will perform advance research work (if any) and summarise his/her research out comes and finalize the dissertation (as per given guideline). At the end of the semester, students have to submit a dissertation and present their findings and progress of the allotted research work.

Guidelines for Dissertation:

The purpose of the dissertation in all semester is to introduce research methodology to the students. It may consist of review of some research papers, development of a laboratory experiment, fabrication of a device, working out some problem related to subject, participation in some ongoing research activity, analysis of data, etc. The work can be carried out in any thrust areas of subject (Experimental or Theoretical) under the guidance of allotted supervisor of the department. The students must submit their dissertation in the department as per the date announced for the submission. Internal assessment of the dissertation work will be carried out by respective supervisor through power point presentation given by candidates during the semester. External assessment of the dissertation work will be carried out by an external examiner (nominated by the Chairperson of the Department) through power-point presentation given by candidates. This load (equivalent to 2 hours per week) will be counted towards the normal teaching load of the teacher.

1. In seven (VII) semester, the assignment/project will be submitted.

2. In VIII, X, IX semester the dissertation will contain a cover page, certificate signed by student and supervisor, table of contents, introduction, Objective, Literature review, methodology, results and discussions conclusion, and references.

- The paper size to be used should be A-4 size.
- The font size should be 12 with Times New Roman.
- The text of the dissertation may be typed in 1.5 (one and a half) space.
- The print out of the dissertation shall be done one or both sides of the paper.

3. The candidate shall be required to submit hard bound copies of dissertation along with a CD/pendrive/respective supervisor e-mail in the department as per the date announced.

4. Dissertation will be evaluated internally by the supervisor allotted to the student during the semester.

5. The candidate will defend her/his dissertation/project work through presentation before the External examiner at the end of semester and will be awarded marks.

6. In case, a student is not able to score passing marks in the dissertation exam, he/she will have to resubmit her/his dissertation after making all corrections/improvements & this dissertation shall be evaluated as above. The candidate is required to submit the corrected copy of the dissertation in hard bound within two weeks after the viva-voce.