M.Sc. (Chemistry)

SYLLABUS FOR TWO-YEAR FULL-TIME PROGRAMME
(Four Semester Course)

(Effective from the Academic Year 2019-20)

Rajiv Gandhi University
Rono Hills, Doimukh 791 112
Arunachal Pradesh

2019

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PREFACE

In compliance with the UGC directives and Rajiv Gandhi University CBCS regulation vide letter no. AC-1465/CBCS/2014/1349 dated 18/03/2015, Department of Chemistry implemented CBCS in the Post Graduate classes from the year 2015. Keeping in view the need to impart value based education; a student friendly syllabus incorporating new ideas and theories in frontier areas of chemistry, Department of Chemistry has revised and updated the Chemistry Syllabus for its Master of Science (M.Sc.) programme as per CBCS format, which is detailed herein. Focus has been given to inculcate interdisciplinary skills that would allow the students both vertical and horizontal mobility in their progression.

Students admitted to this course, must have Major/Honours in Chemistry at degree level (3 Years Course after 10+2) from RGU or any other University recognized by UGC. Candidate must have passed 10+2 (Senior Secondary) or equivalent examination with Mathematics as one of the regular subjects.

The course consists of four semesters with a total of 90 credits with a minimum of 22 credits per semester. Detailed distribution of courses and the corresponding credits are given subsequently. Each semester provides for theory and practical courses. Students are allowed to choose elective courses the different branches of chemistry – Inorganic, Organic and Physical Chemistry. Current course is in line with the vision of RGU for providing a rigorous academic curriculum and a vibrant atmosphere for learning that equips students to solve national and global concerns. These are evident in the emphasis in all courses on fundamentals and on flexibility (20 % flexibility in syllabi mandated through an Academic Council Resolution), in the incorporation of regional, national and global components in the learning objectives.

24th May 2019
Rono Hills, Doimukh

Dr. Rajesh Chakrabarty
Chairman
Board of Post Graduate Studies (BPGS)
Department of Chemistry, RGU

DEPARTMENTAL PROFILE

The Department of Chemistry was established in the year 2011. It marked a humble beginning to impart quality teaching in chemistry and research in frontier areas of chemistry in this region of India. Department of Chemistry, situated in the lush green surroundings on the University Campus, offers programs leading to M.Sc. and Ph.D. degrees.

The Department offers a Two-year M.Sc. programme with specialization in all major areas of chemistry to provide students with the necessary theoretical background and introduction to laboratory methods. In addition to providing a rigorous academic curriculum and a vibrant atmosphere for learning basic and applied chemistry, we aim to produce high-quality graduates who can prove themselves in addressing the challenges in chemistry through research and innovation.

Department is striving to mark its footprint in the diverse areas modern chemical research via its well-trained young faculties. The Department is offering Ph.D. programme in chemistry since 2014. The region being a biodiversity hotspot, there is an immense potential for research and development in the field of natural products and medicinal chemistry. In this regard, we are engaged in sustainably harnessing the vast natural resources and endemic medicinal plants of this region to improve the quality of life of the citizens of the country. The faculties are actively involved in research via sponsored research projects. Since its inception, faculties have been able to receive support for their research projects from various funding agencies – DST (Department of Science & Technology), DBT (Department of Biotechnology), CSIR (Council for Scientific and Industrial Research), UGC (University Grants Commission) and DAE-BRNS (Department of Atomic Energy-Board of Research in Nuclear Sciences).

24th May 2019
Rono Hills, Doimukh

Dr. Rajesh Chakrabarty
Head, Department of Chemistry
Rajiv Gandhi University

REGULATIONS RELATING TO CHOICE BASED CREDIT SYSTEM

Under the Credit Based Semester System (CBSS), the requirement for awarding and conferring a degree is prescribed in terms of number of credits to be completed by the students. Regulations on Choice Based Credit System (CBCS) of Rajiv Gandhi University apply to all postgraduate degree, diploma and certificate programmes awarded and conferred by Rajiv Gandhi University. The CBCS provides choice for students to select from a pool of Open Elective Courses offered by other Departments/Centers/Institutes.

1. COURSES OFFERED BY THE DEPARTMENT

Usually a course refers to a 'paper' and is a component of an academic programme. The Department of Chemistry, RGU offers two-year (4 semesters) M.Sc. programme consisting of **Core Courses**, **Departmental Elective Courses** and **Open Elective Courses**.

NOTE: Each student has to register for one (1) open elective course during the III Semester offered by other Departments/Centers/Institutes. Students are not allowed to register for open elective course offered by the parent department.

2. REGISTRATION PROCESS FOR OPEN ELECTIVE COURSE

- ***STEP 1***: Immediately after joining M.Sc. Programme, the student shall fill up **two copies** of Open Elective Course Application Form (Annexure II). **Student Advisor** (a Faculty from the Department) will advise and assist in choosing a suitable Open Elective Course.

- ***STEP 2***: Copy 1 to be submitted to Head, Department of Chemistry and Copy 2 to be submitted to Department where the student is applying for Open Elective Course.

NOTE: Late registration for Open Elective Courses shall be allowed up to two weeks after the commencement of the semester.

3. WITHDRAWAL PROCESS FOR OPEN ELECTIVE COURSE

Withdrawal from an Open Elective Courses shall be allowed within two weeks from the date of commencement of classes.

4. COURSE CODING

- The courses offered by the department carry a three-letter departmental code (CHE) that is followed by a single-letter code like; **C** for Core, **E** for Departmental Elective and **O** for Open Elective. Next three-digit number refers to course code series; **4XX** for M.Sc. First Year while **5XX** for M.Sc. Second Year.

- The number of credits is given in the form **L : T : P : C**, where **L** indicates the number of contact hours of lecture, and **T** the number of contact hours for tutorials, **P** stands for laboratory credits and **C** for total credit per course. Each lecture credit corresponds to one lecture hour per week, while each laboratory credit corresponds to a 2-hour laboratory class. For example, 3 : 1 : 0 : 4 credits indicates that the course would have 3 lecture hours along with one tutorial session and no laboratory each week, while 1 : 1 : 2 : 4 credits indicates a course with one lecture hour, one tutorial session and two 2-hour laboratory.

5. GRADE POINT AND GRADE LETTER

% of Marks	Grade Point	Grade Letter	Division
90 – 100 %	10	O (Outstanding)	First
80 – less than 90 %	9	A+ (Excellent)	First
70 – less than 80 %	8	A (Very Good)	First
60 – less than 70 %	7	B+ (Good)	First
50 – less than 60 %	6	B (Average)	Second
45 – less than 50 %	5	P (Pass)	Pass
44 % and less	0	F (Fail)	Fail
Absent	0	AB (Absent)	

6. SEMESTER GRADE POINT AVERAGE (SGPA)

Semester Grade Point Average (SGPA) is the sum of the products of the course credit and grade points scored by a student divided by the sum of all course credits in a semester. It can be calculated in the following manner:

$$SGPA\left(S_i\right) = \frac{\sum (C_i \times G_i)}{\sum C_i}$$

Where, C_i is the number of credits of the i^{th} course and G_i is the grade point scored by the student in the i^{th} course. For example, an illustration of computation of SGPA is shown below:

Courses in the Semester	Mark obtained (Internal Assessment + End semester exam)	Grade Letter	Grade Point (G)	Credit (C)	Credit Point Σ□□
Course 1	78	A	8	3	3 × 8 = 24
Course 2	65	B+	7	3	3 × 7 = 21
Course 3	82	A+	9	4	4 × 9 = 36
Course 4	49	P	5	4	4 × 5 = 20
Course 5	53	B	6	5	5 × 6 = 30
				21	**131**

Thus,

$$SGPA = \frac{131}{21} = 6.23$$

7. CUMULATIVE GRADE POINT AVERAGE (CGPA)

Cumulative Grade Point Average (CGPA) is the sum of the products of the total number of credits of all courses taken by a student in a semester with the SGPA in that semester divided by the total number of credits of all courses taken in all four semester. It can be calculated in the following manner:

$$CGPA = \frac{\sum (C_i \times S_i)}{\sum C_i}$$

Where, S_i is the SGPA of the i^{th} semester and C_i is the number of credits in that semester.

For example, an illustration of computation of CGPA is shown below:

	Semester I	**Semester II**	**Semester III**	**Semester IV**
Total Credit	21	21	21	27
SGPA	7.8	5.8	6.3	8.0

Thus,

$$CGPA = \frac{21 \times 7.8 + 21 \times 5.9 + 21 \times 6.3 + 27 \times 8.0}{90} = 7.07$$

SALIENT FEATURES OF THE COURSE

- The listing of each course consists of the semester, course code, course title, the number of credits, the set of topics and the list of recommended books.

- Each course of theoretical nature with 4 credits consists of 4 modules/units while each practical paper is of 5 credits.

- In terms of marks, each course is of 100 marks; 20 marks for internal assessment and 80 marks in final examination. Each module/unit in a course of theoretical nature carries 20 marks.

- Each student of M.Sc. (Semester III and IV) shall have to opt for the respective Departmental Elective Course (I, II, III and IV) of their chosen branch of specialization.

- Each student of M.Sc. Semester IV shall have to opt for project work or advanced practical and literature survey. Project work would be assigned on merit basis and total number of students for project would be decided at the department level.

- For project work, the area of the work would be to be decided by the advisor. On completion of the project work, students have to submit the work in the form of a dissertation followed by oral presentation in the presence of faculty members and external expert(s).

- Each student of M.Sc. (Chemistry) shall have to complete a SWAYAM course of 4 Credit (8-12 Weeks) in lieu of Open Elective Course during the Semester III.

  or

  1 (one) audit course (8-12 Weeks) from SWAYAM platform.

  For audit course, students will have the flexibility to register for the course any time during the M.Sc. (Chemistry) course duration. However, they have to submit the SWAYAM course completion certificate before the End-semester examination of IV Semester.

- Students will have the option to opt for a SWAYAM course of 4 Credit (8-12 Weeks) in lieu of Open Elective Course during the Semester III.

- The members recommended to appoint a departmental coordinator for coordinating the SWAYAM courses.

- Members recommended that, the SWAYAM course to be opted by the students would be decided at the departmental level and be placed in the Academic Council for approval.

COURSE STRUCTURE

Semester	Core Courses			Elective Courses			Open Elective Courses / SWAYAM Courses			Total Credits
	No. of Papers	Credits (L + T/P)	Total Credits	No. of Papers	Credits (L + T/P)	Total Credits	No. of Papers	Credits (L + T/P)	Total Credits	
I	5	16 + 6	22	Nil		0	Nil		0	22
II	5	16 + 6	22	Nil		0	Nil		0	22
III	3	8 + 6	14	1	4	4	1	4	4	22
IV	1	4	4	3	8 + 12	20			0	24
TOTAL			62			24			4	**90**

Scheme of Examination

Course Code	Course Title	Nature of Course	Maximum Marks			Credit Distribution	Credit	Total Credit
			Sessional	Terminal	Total	L : T : P		
Semester I								
CHEC 401	Inorganic Chemistry I	Core	20	80	100	3 : 1 : 0	4	**22**
CHEC 402	Organic Chemistry I	Core	20	80	100	3 : 1 : 0	4	
CHEC 403	Physical Chemistry I	Core	20	80	100	3 : 1 : 0	4	
CHEC 404	Quantum Chemistry	Core	20	80	100	3 : 1 : 0	4	
CHEC 405	Physical Chemistry Laboratory	Core	20	80	100	0 : 0 : 6	6	
Semester II								
CHEC 406	Inorganic Chemistry II	Core	20	80	100	3 : 1 : 0	4	**22**
CHEC 407	Organic Chemistry II	Core	20	80	100	3 : 1 : 0	4	
CHEC 408	Physical Chemistry II	Core	20	80	100	3 : 1 : 0	4	
CHEC 409	Molecular Spectroscopy	Core	20	80	100	3 : 1 : 0	4	
CHEC 410	Organic Chemistry Laboratory	Core	20	80	100	0 : 0 : 6	6	
Semester III								
CHEC 501	Materials Chemistry	Core	20	80	100	3 : 1 : 0	4	**22**
CHEC 502	Applications of Molecular Spectroscopy	Core	20	80	100	3 : 1 : 0	4	
CHEC 503	Organometallic & Heterocyclic Chemistry	Core	20	80	100	3 : 1 : 0	4	
CHEC 504	Inorganic Chemistry Laboratory	Core	20	80	100	0 : 0 : 6	6	
	Open Elective Course / SWAYAM Course	Open Elective					4	

Semester IV								
CHEC 505	Biochemistry	Core	20	80	100	3 : 1 : 0	4	24
CHEE 5X1	Elective Course I	Elective	20	80	100	3 : 1 : 0	4	
CHEE 5X2	Elective Course II	Elective	20	80	100	3 : 1 : 0	4	
CHEE 5X3 ***OR*** CHEE 551	Elective Course III ***OR*** Elective Course IV: Project Dissertation	Elective	20	80	100	0 : 0 : 12	12	
Online Audit Course through SWAYAM Platform		Open Elective						

**Students will have to opt one course out of CHEE 5X3 and CHEE 551.*

Departmental Elective Courses

Specialization	Course Code	Course Title	Maximum Marks			Credit Distribution	Credit
			Sessional	Terminal	Total	L : T : P	
Inorganic	CHEE 511	Elective Course I: Inorganic Reaction Mechanisms	20	80	100	3 : 1 : 0	4
	CHEE 512	Elective Course II: Bioinorganic Chemistry	20	80	100	3 : 1 : 0	4
	CHEE 513 ***OR*** CHEE 551	Elective Course III: Advanced Inorganic Chemistry Laboratory & Literature Survey ***OR*** Elective Course IV: Project Dissertation	20	80	100	0 : 0 : 12	12
Organic	CHEE 521	Elective Course I: Organic Synthesis II	20	80	100	3 : 1 : 0	4
	CHEE 522	Elective Course II: Natural Products and Medicinal Chemistry	20	80	100	3 : 1 : 0	4
	CHEE 523 ***OR*** CHEE 551	Elective Course III: Advanced Organic Chemistry Laboratory & Literature Survey ***OR*** Elective Course IV: Project Dissertation	20	80	100	0 : 0 : 12	12

Physical	CHEE 531	Elective Course II: Polymer Chemistry	20	80	100	3 : 1 : 0	4
	CHEE 532	Elective Course III: Advanced Chemical Kinetics and Photochemistry	20	80	100	3 : 1 : 0	4
	CHEE 533 ***OR*** CHEE 551	Elective Course III: Advanced Physical Chemistry Laboratory & Literature Survey ***OR*** Elective Course IV: Project Dissertation	20	80	100	0 : 0 : 12	12

**Students will have to opt one course out of CHEE 513/ CHEE 523 / CHEE 523 and CHEE 551.*

Open Elective Courses

Semester	Course Code	Course Title	Maximum Marks			Credit Distribution	Credit
			Sessional	Terminal	Total	**L : T : P**	
Semester III	CHEO 541	Environmental and Green Chemistry	20	80	100	3 : 1 : 0	4
	CHEO 542	Bioanalytical and Medicinal Chemistry	20	80	100	3 : 1 : 0	4
	CHEO 543	Applications of Molecular Spectroscopy	20	80	100	3 : 1 : 0	4

These open elective courses of interdisciplinary nature are intended to be studied by students from other departments.

SEMESTER I

CHEC 401 Inorganic Chemistry I

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: In this introductory course on inorganic chemistry, students will be able to understand the importance of symmetry and group theory, main group chemistry and inorganic cages and clusters.

Learning outcome: Students will be able to explain/describe/rationalize molecular structure and bonding using group theory, inorganic cages and clusters.

UNIT I: Molecular Symmetry and Group Theory

Symmetry elements and operations. Group and its characteristics, subgroup, classes, similarity transformations. Product of symmetry operations, equivalent atoms and equivalent symmetry elements. Relation between symmetry elements and operations, classes of symmetry operations. Matrix representation of groups, reducible and irreducible representations. Orthogonality theorem, properties of irreducible representations, character tables and their construction. Mulliken notations.

UNIT II: Applications of Group Theory

Direct product representation, projection operator and symmetry adapted linear combination (SALC), symmetry selection rules for IR, Raman and electronic spectra.
Hybrid orbital and hybridization in polyatomic molecules, construction of hybrid orbitals for sigma & π-bonding (e.g. D_{3h}, D_{4h}, T_d, O_h). Molecular Orbital Theory: LCAO-MO approach; Construction of MO diagrams of polyatomic molecules (e.g. BeH_2, H_2O, BH_3, NH_3, CH_4) including coordination complexes (O_h and T_d).

UNIT III: Structure and Energetics in Metallic and Ionic solids

A brief introduction to crystal systems: Lattices, unit cells, space groups. Packing of spheres: Hexagonal and cubic closed packing, Tetrahedral and octahedral holes in close packed structure; radius ratios in determining structure type among ionic solids. Characteristic structure types of ionic solids: CsCl, NaCl, Spalerite and Wurtzite types of ZnS, fluorite and anti-fluorite, nickel arsenide, $CdCl_2$, CdI_2, rutile, perovskite and spinels. Lattice enthalpy, consequences of lattice enthalpy.

UNIT IV: Inorganic Cages and Clusters

Structure and bonding in polyhedral boranes, carboranes, metalloboranes and metallocarboranes, *styx* notation; Wade's rule; electron count in polyhedral boranes; synthesis of polyhedral boranes. Synthesis, structure and bonding in borazines, phosphazenes, sulphur-nitrogen compounds, siloxanes, iso- and hetero-poly anions. Structure and chemistry of silicates, aluminosilicates, zeolites and clays.

Recommended Books

1. Cotton, F. A., *Chemical Applications of Group Theory*, 3rd Ed., Wiley India, New Delhi (2008).
2. Reddy, K. V., *Symmetry and Spectroscopy of Molecules*, 2nd Ed., New Age International Publishers, New Delhi (2009).
3. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 5th Ed., Pearson Education, Essex (2018).
4. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 6th Ed., Oxford University Press, New Delhi (2015).
5. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education India, New Delhi (2008).
6. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education India, New Delhi (2006).

Further Reading

1. Carter, R. L., *Symmetry and Group Theory*, Wiley India, New Delhi (2009).
2. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2007).

SEMESTER I

CHEC 402 Organic Chemistry I

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: In this course on organic chemistry, students will be introduced to conceptual organic chemistry, stereochemistry of organic molecules, reaction mechanisms and the intermediates.

Learning outcome: Students will be able to appreciate/demonstrate/explain the unique features of organic reactions mechanism, reaction intermediates and stereochemistry, and solve related problems.

UNIT I: Basic Stereochemistry

Stereoisomerism in organic compounds: brief introduction of geometrical and optical isomerism.

Interconversions of projection formulae, Conformational analysis of simple cyclic and acyclic systems, butane- gauche and 1,3-diaxial interactions and their influences in stability of molecules.

Optical purity, optical activity in absence of chiral centre: chiral axis, chiral plane and helical chirality.

Asymmetry and dissymmetry: Concept of stereogenic, chirotopic and achirotopic centres; prochirality (*Re*- & *Si* face), prosterioisomerism; homotopic and heterotopic faces; diastereomerism in acyclic and cyclic systems.

UNIT II: Conceptual Organic Chemistry

Review of basic concepts: inductive effect, electromeric effect, resonance effect, hyperconjugation, resonance. Aromaticity: Huckel's rule, aromatic, non-aromatic, antiaromatic, homoaromatic compounds, *n*-annulenes.

Applications of acid-base concept: HSAB and its applications.

Review of reaction mechanisms: thermodynamic and kinetic requirement of reactions, Hammond postulate, intermediate and transition states, kinetically and thermodynamically controlled products and reactions, methods of determination of mechanism, primary and secondary kinetic isotope effect, linear free energy relationships and their application (Hammett equation and modifications).

UNIT III: Ionic Reaction Intermediates

Carbocation: Generation, structure and reactivity, classical and non-classical carbocations, neighbouring group participation and rearrangements in acyclic, monocyclic and bicyclic systems.

Carbanions: Generation, structure and reactivity. Organolithium, organomagnesium, organozinc, organocopper reagents.

Enolates: Themodynamic versus kinetic enolates, enolate equivalent and enamines: Application in carbon-carbon bond formation and other reactions. Cram's rule, Felkin-Anh model, Zimmerman-Traxler model.
Ylides: Chemistry of phosphorous and sulfur ylides – Wittig reaction: stabilized and non-stabilised ylides, related reactions, Petersen olefination.

UNIT IV: Non-ionic Reaction Intermediates

Free radicals: Generation, structure, stability and reactions, radical initiator, cage effects, radical cations and radical anions, application of tributyltinhydride/AIBN, Hoffmann-Loeffler-Freytag reaction and Barton reaction.
Carbenes: Formation, structure and stability, singlet and triplet states, Reimer-Tiemann and other reactions involving carbene intermediate.
Nitrenes: Generation & structure, reactions of nitrenes and related electron deficient nitrogen intermediates.
Arynes: Generation, structure and stability, rearrangement reactions, S_NAr mechanism.

Recommended Text Books

1. Smith, M. B.; March, J., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th Ed., Wiley India, New Delhi (2015).
2. Greeves, N.; Clayden, J.; Warren, S., *Organic Chemistry*, 2nd Ed., Oxford University Press, New Delhi (2012).
3. Nasipuri, D. *Stereochemistry of Organic Compounds: Principles and Applications*, 3rd Ed., New Age International Publishers, New Delhi (2018).

Further Reading

1. Smith, M. B., *Organic Synthesis*, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).
2. Sengupta, S., *Basic Stereochemistry of Organic Molecules*, 2nd Ed., Oxford University Press, New Delhi (2018).
3. Kalsi, P. S., *Stereochemistry: Conformation and Mechanism*, 10th Ed., New Age International Publishers, New Delhi (2019).

SEMESTER I

CHEC 403 Physical Chemistry I

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: In this course on physical chemistry, students will be introduced to fundamentals chemical thermodynamics, chemical kinetics and surface chemistry.

Learning outcomes: Students will be able to understand and explain the fundamentals of chemical thermodynamics, chemical kinetics and surface chemistry and apply the concepts to solving problems.

UNIT I: Chemical Thermodynamics

Brief resume of law of thermodynamics; Gibbs and Helmholtz free energy functions and their significance. Thermodynamic criteria for the processes in terms of entropy change, internal energy change, enthalpy and free energy (Gibbs and Helmholtz) change. Gibbs – Helmholtz equation and its utility in thermodynamics of reaction.
Fugacity and activity and their variation with temperature and pressure. Graphical method for the determination of fugacity; fugacity of van der Waals gases.
Partial molar quantities and its physical significance; Partial molar free energy (chemical potential) and its variation with temperature and pressure; Gibbs-Duhem equation.
Gibbs free energy and entropy of mixing of ideal gases; partial molar volumes; method of determination of partial molar volumes. Thermodynamic description of phase transitions and Clapeyron-Claussius equation.

UNIT II: Non–Equilibrium Thermodynamics

Difference between equilibrium and non- equilibrium thermodynamics, Postulates of non-equilibrium thermodynamics; Curie-Prigogine principle and microscopic reversibility. Onsagar's relations: thermodynamic and kinetics point of view; phenomenological laws.
Entropy of irreversible processes: Clausius inequality; entropy production due to heat flow, mass flow, chemical reactions and electrochemical reactions; rate of entropy productions-generalized fluxes and forces; thermodynamic forces and fluxes; relation between forces and fluxes; Thermoelectric phenomenon: Peltier, Seebeck and Thompson effect. Relation between chemical potential and thermodynamic potentials.

UNIT III: Chemical Kinetics I

Kinetics of complex reactions: consecutive, side and opposing reactions (first order only); steady state approximation and kinetics of some selected reactions.
Chain reactions: general treatment and explanation of explosions; reaction mechanism and kinetics of H_2-Br_2 reaction and pyrolysis of alkane.
Enzyme catalysis: mechanism and kinetics of enzyme catalysis reaction; oscillatory reactions: mechanism and kinetics. Reactions in flow systems; kinetics of fast reaction.

UNIT IV: Surface Chemistry

Adsorption from solution: surface tension and surface free energy, application of surface tension, capillary action: Young-Laplace equation; formation of bubbles: Kelvin equation. Capillary condensation; adsorption in micropores and hysteresis loop.

Adsorption and surface tension: Gibbs adsorption equation; surface active and surface inactive materials.

Formation of surface films on liquids; electrical aspects of surface chemistry; electro kinetic phenomena; the structure of electrical double layer; zeta potential and colloidal stability.

Adsorption of gases on solid surface: Thermodynamics of adsorption; application of adsorption; factors affecting adsorption.

Adsorption isotherms: Langmuir isotherm and BET isotherm; determination of surface area of an adsorbent (Langmuir and BET equation); isosteric enthalpy of adsorption.

Catalytic activity at surfaces: mechanism of surface reaction; Langmuir-Hinshelwood and Eley-Rideal model; kinetic effects of surface heterogeneity and interactions. Kinetics of heterogeneous catalysis: unimolecular and bimolecular surface reactions.

Recommended Books

1. Atkins, P. W.; de Paula, J.; Keeler, J., *Physical Chemistry,* 11th Ed., Oxford University Press, New Delhi (2018).
2. Silbey, R. J.; Alberty, R. A.; Bawendi, M. G., *Physical Chemistry*, 4th Ed., Wiley India, New Delhi (2006).
3. Levine, I. N., *Physical Chemistry,* 6th Ed. McGraw Hill Education, New Delhi (2011).
4. Kalidas, C.; Sangaranarayanan, M. V., *Non-Equilibrium Thermodynamics-Principles and Applications*, Macmillan Publishers India, New Delhi (2002).
5. Laidler, K. J., *Chemical Kinetics*, 3rd Ed., Pearson Education, New Delhi (2011).
6. Kapoor, K. L., *A Textbook of Physical Chemistry: States of Matter and Ions in Solution*, Vol. I, 6th Ed., McGraw Hill Education India (2019).
7. Kapoor, K. L., *A Textbook of Physical Chemistry: Thermodynamics and Chemical Equilibrium*, Vol. II, 6th Ed., McGraw Hill Education India (2019).

Further Reading

1. Puri, B. R.; Sharma, L. R.; Pathania, M. S., *Principles of Physical Chemistry*; 47th Ed, Vishal Publishing, New Delhi (2017).
2. Lebon, G.; Jou, D.; Casas-Vazquez, J., *Understanding Non-equilibrium Thermodynamics: Foundations, Applications, Frontiers,* Springer, Heidelberg (2008).
3. Prigogine, I., *Introduction to Thermodynamics of Irreversible Processes*, 3rd Ed., Wiley (1968).
4. Adamson, A. W.; Gast, A. P., *Physical Chemistry of Surfaces,* 6th Ed, Wiley India, New Delhi (2011).
5. Shaw, D. J., *Introduction to Colloid and Surface Chemistry*, 4th Ed, Butterworths-Heinemann, Oxford (1992).
6. Moudgil, H. K., *Textbook of Physical Chemistry,* PHI Learning, New Delhi (2010).

SEMESTER I

CHEC 404 Quantum Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: To introduce students to the fundamental principles and modern aspects of quantum chemistry.

Learning outcome: Students will be able to explain the theoretical basis of quantum chemistry, and critically examine/interpret the theories/principles, compare various approximate formalisms and their validity in explaining experimental phenomena.

UNIT I: Origin of Quantum Mechanics

Mathematical concepts: differential equation, integration, vectors, matrix and determinants.
Brief review on the failure of classical mechanics (Planck's quantum theory, photoelectric effect, wave particle duality, uncertainty principle).
Time-independent Schrödinger equation and properties of wave functions.
Postulates of quantum mechanics; normalization and orthogonality; quantum mechanical operators; properties of operators; eigenvalues and eigenfunctions; setting up of operators for different observables; orbital angular momentum operators; Hermitian operators; Schmidt-orthogonalization technique.

UNIT II: Wave Mechanics of Some Simple Systems

Particle in a one dimensional box; characteristics of wave functions; quantization of energy levels; zero point energy and Heisenberg uncertainty principle; probability distribution functions and nodal properties.
Three dimensional box; separation of variables; degree of degeneracy; concept of tunnelling.
Qualitative treatment of simple harmonic oscillator model of vibrational motion: Setting up of Schrödinger equation and discussion of solution and wave functions; normalization of wave functions. Vibrational energy of diatomic molecules and zero-point energy.
Rigid rotator model of rotation of diatomic molecule: Schrödinger equation; transformation to spherical polar coordinates. Separation of variables; spherical harmonics and discussion of solution.
Qualitative treatment of hydrogen atom and hydrogen-like ions: setting up of Schrödinger equation in spherical polar coordinates; radial part; quantization of energy (only final energy expression). Average, root mean square and most probable distances of electron from nucleus.

UNIT III: Application of Quantum Mechanics I

Variation theorem and linear variation functions; first order time-independent perturbation theory for non-degenerate states; application of variation treatment and perturbation treatment to the helium atom. Born-Oppenheimer approximation, Hartree and Hartree-Fock Self-Consistent Field method. Slater determinant.

Hückel electron theory and extended Hückel MO theory and their application to ethylene, butadiene, allyl system and benzene.

UNIT IV: Application of Quantum Mechanics II

Semi-empirical and bound-state *ab* initio quantum mechanical and density functional calculations, understanding of basis set types and sizes, computational scalability, Hartree-Fock and Post-Hartree-Fock calculations for determining electronic energies and associated molecular properties, electronic structure and thermochemical properties, geometry optimization, study of reaction mechanism, transition-state optimizations.

Recommended Books

1. Chandra, A. K., *Introductory Quantum Chemistry*, 4th Ed., McGraw Hill Education India, New Delhi (2017).
2. Levine, I. N., *Quantum Chemistry*, 7th Ed., Pearson Education India, New Delhi (2016).
3. McQuarrie, D. A., *Quantum Chemistry*, Viva Books, New Delhi (2016).
4. Lewers, E. G., *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*, 2nd Ed., Springer, New York (2011).
5. Jensen, F., *Introduction to Computational Chemistry*, 3rd Ed., Wiley-Blackwell, New Jersey (2017).

Further Reading

1. Sen, B. K., *Quantum Chemistry Including Spectroscopy*, 2nd Ed., Kalyani Publishers, New Delhi (2004).
2. Atkins, P. W., Friedman R. S., *Molecular Quantum Mechanics*, 5th Ed., Oxford University Press, New Delhi (2012).
3. Prasad, R. K., *Quantum Chemistry*, 4th Ed., New Age International Publishers, New Delhi (2010).

SEMESTER I

CHEC 405 Physical Chemistry Laboratory

Contact Hours per week: 6
Credits: 6
Terminal Examination Duration: 8 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This core laboratory course introduces students to experimental physical chemistry and computational chemistry. Part A is involved with basic physical chemistry such as chemical kinetics, surface chemistry, thermodynamics, spectrophotometry etc. Part B experiments are aimed to develop computational chemistry skills and spectral interpretation of organic compounds.

Learning outcome: From this course, the students will understand physical chemistry from experimental point of view. Moreover, they will learn computational chemistry methods.

PART A: Marks: 60

Physical Chemistry Experiments

At least 10 (ten) experiments must be performed from among the following:

1. To determine the rate constant of acid catalyzed hydrolysis of ester at two / three different temperatures and to calculate the value of activation energy of the reaction.
2. To determine the rate constant of hydrolysis of ethyl acetate with NaOH.
3. To investigate the reaction between acetone and iodine in presence of an acid and to determine the order with respect to each reactant.
4. To investigate the autocatalytic reaction between potassium permanganate and oxalic acid.
5. To determine the molar mass of a polymer (polystyrene) by viscometry technique.
6. To determine the critical micelle concentration of a sample surfactant by surface tension method.
7. To compare the cleansing powers of two samples of detergent by surface tension method.
8. To study the distribution of benzoic acid between benzene and water and hence show that benzoic acid dimerizes in benzene.
9. To determine molar conductivity of a strong electrolyte at different concentrations and verify Debye-Hückel-Onsager equation.
10. To determine the equivalent conductance of a weak electrolyte at infinite dilution using Kohlrausch law.
11. To determine the strength of the components of the following mixtures by conductometric titration: (i) hydrochloric acid and acetic acid; (ii) hydrochloric acid and potassium chloride and (iii) sulphuric acid and copper sulphate.
12. To determine the dissociation constant of acetic acid by pH determination of acetic acid and sodium acetate using Henderson equation.
13. To determine the strength of HCl and CH_3COOH in a given mixture by pH metric titration.
14. To determine the strength of HCl and CH_3COOH in a given mixture by potentiometric titration.

15. To verify Lambert-Beer law and hence to determine the concentration of solutions like $KMnO_4$/ methyl red/ methyl orange spectrophotometrically.
16. To determine the composition of iron-salicylic acid complex spectrophotometrically by Job's method of continuous variation.
17. To investigate the adsorption of oxalic acid from aqueous solutions by activated charcoal and examine the validity of Freundlich isotherm.
18. To determine critical solution temperature (CST) of phenol and water system and to study the effect of 1 % NaCl on the CST.

PART B: Marks: 20

Computational Calculations

1. To perform theoretical calculations using a computer on
   (a) Least square fitting and plotting linear and exponential graphs.
   (b) Potential energy diagram of hydrogen molecule ion.
   (c) Charge density distribution and shapes of *s* and *p* orbitals.

2. To plot for Maxwell's speed distribution formula in speed and translational energy term and calculate the fraction of molecules in a given speed range by numerical integration.

3. *Ab-initio* calculations of organic and inorganic molecules using GAUSSIAN software.

4. Spectral interpretation of organic compounds via UV, IR Mass and NMR spectra

Recommended Books

1. Halpern, A. M.; McBane, G. C., *Experimental Physical Chemistry: A Laboratory Textbook*, W. H. Freeman, New York (2006).
2. Viswanathan, B.; Raghavan, P. S., *Practical Physical Chemistry*, Viva Books, New Delhi (2014).
3. Yadav, J. B., *Advanced Practical Physical Chemistry*, Krishna Prakashan, Meerut (2015).
4. Lewers, E. G., *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*, 2nd Ed., Springer, New York (2011)
5. Jensen, F., *Introduction to Computational Chemistry*, 3rd Ed., Wiley-Blackwell, New Jersey (2017).

SEMESTER II

CHEC 406 Inorganic Chemistry II

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: To Introduce students to the chemistry of transition elements and fundamental aspects of supramolecular chemistry.

Learning outcome: Students will be able to apply their knowledge of *d*- and *f*-block elements in explaining, interpreting and critically examining bonding, structure, reactivity, magnetic and spectral properties. Students will also learn about the various aspects of supramolecular chemistry.

UNIT I: Bonding in Transition Metals

Crystal field theory of bonding in octahedral, JT-distorted octahedral, square planar, square pyramidal, trigonal bipyramidal, and tetrahedral complexes; CFSE for d^1 to d^{10} systems, pairing energy, low-spin and high-spin complexes.

Ligand Field Theory (LFT) and molecular orbital (MO) theory of selected octahedral and tetrahedral complexes; thermodynamic aspects of LFSE.

UNIT II: Magnetic Properties of *d*- and *f*-block Metal Complexes

Magnetic susceptibility, Measurement of magnetic susceptibility using Gouy and Faraday methods. Spin orbit coupling, spin and orbital contributions to the magnetic moment, quenching of orbital angular momentum. Spin crossover complexes; magnetic properties of lanthanides and actinides.

Effect of Temperature on magnetic moment: Curie, Curie-Weiss laws. Brief review of different types of cooperative magnetic behavior.

UNIT III: Electronic Spectra of *d*- and *f*-block Metal Complexes

Electronic Spectra of complexes: Microstates and term symbols, term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling, *d*-*d* transition.

Interpretation of electronic spectra of complexes: Orgel diagrams, Tanabe-Sugano diagrams, calculation of Dq, B and β (Nephelauxetic ratio) values, charge transfer spectra.

Spectral properties of Lanthanide and Actinide metal complexes.

UNIT IV: Supramolecular Chemistry

Origin of supramolecular chemistry. Concepts and terminology of supramolecular chemistry. Types of supramolecular interactions (Hydrogen bonding, van der Waals interaction, π-stacking, CH-π, anion-π interaction).

Host-guest Chemistry: macrocyclic effect and their thermodynamic origin, Step-wise and overall binding constant in host-guest chemistry, kinetic and thermodynamic selectivity.

Binding of organic and inorganic cationic, anionic, ion pair and neutral guest molecules with host molecules. Self-assembly: Definitions and basic concepts of self-assembly, self-assembly using metal templates. Applications of self-assembled molecules.

Recommended Books

1. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 5th Ed., Pearson Education, Essex (2018).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 6th Ed., Oxford University Press, New Delhi (2015).
3. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education India, New Delhi (2008).
4. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education India, New Delhi (2006).
5. Steed, J. W.; Turner, D., R.; Wallace, K. J., *Core Concepts in Supramolecular Chemistry and Nanochemistry*, John Wiley & Sons, West Sussex (2007).
6. Steed, J. W.; Atwood, J. L., *Supramolecular Chemistry*, 2nd Ed., John Wiley & Sons, West Sussex (2009).

Further Reading

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2007).
2. Ariga, K.; Kunitake, T., *Supramolecular Chemistry: Fundamentals and Applications*, Springer, Heidelberg (2006).
3. Lehn, J.-M., *Supramolecular Chemistry: Concepts and Perspectives*, Wiley India, New Delhi (2014).
4. Figgis, B. N.; Hitchman, M. A., *Introduction to Ligand Field Theory and Its Applications*, Wiley India, New Delhi (2010).

SEMESTER II

CHEC 407 Organic Chemistry II

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course will enable the students to comprehend various types of organic reactions, their mechanisms and applications.

Learning outcome: Through this course students will acquire the detailed knowledge on substitution, elimination, addition, oxidation and reduction, photochemical and pericyclic reactions**.**

UNIT I: Substitution, Elimination and Addition Reactions

Substitution Reactions: Mechanism and reactivity of aromatic, aliphatic, nucleophilic substitution reaction, orientation and reactivity in aromatic electrophillic substitution reactions.
Elimination Reactions: Mechanism, orientation and reactivity, dehydration of alcohols, Shapiro reaction, conversion of epoxide to olefins**,** dehalogenation of vicinal halide. Substitution vs. elimination, nucleophile vs. base.
Addition Reactions: Mechanism and stereochemical aspects of addition reactions in carbon-carbon multiple bonds.

UNIT II: Oxidation

Oxidation: Metal and non-metal based oxidations of alcohols to carbonyls (Chromium, manganese, aluminium, silver, DMSO and hypervalent iodine. Oxidation of phenols: Fremy's salt, alkenes to epoxides: via halohydrin, peroxides/per acids based, Sharpless asymmetric epoxidation; alkenes to diols (Manganese, osmium based), Prevost reaction and Woodward modification; oxidation of alkyl or alkenyl fragments: selenium dioxide, ketones to ester/lactones: Baeyer-Villiger oxidation.

UNIT III: Reduction

Reduction: Catalytic hydrogenation (Heterogeneous: Palladium/ Platinum/ Rhodium/ Nickel etc; Homogeneous: Wilkinson); metal-liquid ammonia processes: Birch reduction, Pinacol formation etc.; stereo selection and mechanism of the following reagents: Lithium aluminium hydride, L-selectride, K-selectride, Sodium borohydride, DIBAL, sodium cyanoborohydride, Alkyl borane, non-metallic reducing agents: diimide.

UNIT IV: Photoorganic and Pericyclic Reactions

Photoorganic Chemistry: cis-trans isomerisation, Norrish type I & II reaction, photoreduction of ketones, Paterno-Buchi reaction, Di- π-methane and Di-π-methane type rearrangement.
Introduction, types: electrocyclic, cycloaddition and sigmatotropic reaction; 1,3-dipolar addition, Ene reaction.

Introduction, types: electrocyclic reaction, cycloaddition, 1,3-dipolar addition, chelotropic reactions, sigmatotropic and group transfer reaction: Ene reaction, selection rules, general orbital symmetry rules.

Recommended Text Books

1. Smith, M. B.; March, J., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 7th Ed., Wiley India, New Delhi (2015).
2. Smith, M. B., *Organic Synthesis*, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).
3. Greeves, N.; Clayden, J.; Warren, S., *Organic Chemistry*, 2nd Ed., Oxford University Press, New Delhi (2012).

Further Reading

1. Carruthers, W., *Modern Methods of Organic Synthesis*, 4th Ed., Cambridge University Press, New Delhi (2005).
2. Zweifel, G. S.; Nantz, M. H.; Somfai, P., *Modern Organic Synthesis: An Introduction*, 2nd Ed., Wiley-Blackwell, New York (2017)

SEMESTER II

CHEC 408 Physical Chemistry II

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: In this course on physical chemistry, students will be able to understand the fundamental aspects of statistical thermodynamics, chemical kinetics and electrochemistry.

Learning outcomes: Students will be able to describe/examine the concepts and theories of statistical thermodynamics, chemical kinetics and electrochemistry and apply the concepts to solving problems.

UNIT I: Statistical Thermodynamics

Concepts of statistical thermodynamics, entropy and thermodynamic probability. Different types of ensembles, ensemble averaging; Stirling approximation.

Distribution laws: Maxwell–Boltzmann, Fermi–Dirac and Bose–Einstein; limitation of applicability of various distribution laws.

Partition functions and its properties, thermodynamic properties in terms of partition functions, evaluation of translational, rotational, vibrational, electronic and nuclear partition functions; law of equipartition of energies; heat capacity.

Molecular partition functions and its importance; determination of thermodynamic properties of a monoatomic gas.

UNIT II: Chemical Kinetics II

Kinetic control and thermodynamic control of reaction; theories of reaction rate: Arrhenius theory; simple collision theory (SCT); steric factor, activated complex theory (ACT); thermodynamics of reaction rate and entropy of activation.

Theories of unimolecular reactions: Lindemann mechanism and Hinshelwood treatment.

Reaction in solution: diffusion controlled and chemically controlled reaction; factors affecting reaction rate in solution; effect of solvent and ionic strength on the rate constant: primary and secondary salt effect; effect of dielectric constant of the medium on the rate of reaction in solution.

UNIT III: Electrochemistry

Fugacity and activity of electrolytes; mean ionic activity; mean ionic activity coefficient and ionic strength.

Free energy change due to ion-solvent interaction: Born model; electrical double layer: Helmholtz–Perrin model; The basic electrodic equation: Butler-Volmer equation; over potential.

Ion–ion interaction: Debye-Hückel equation (derivation, validity and limitations), extended Debye-Hückel equation.

Ion association and effect of conductance: Debye-Hückel-Onsager equation; the random walk model of ionic diffusion: Einstein-Smoluchowski relation.

UNIT IV: Macromolecules

Brief overview of polymers: Classification and types of polymers. Concept and types of molecular weight; distribution of molecular weight in polymers; significance of molecular weight; degree of polymerization and chain length.

Methods of determining molecular weights of macromolecules: End group analysis; osmometry, viscometry and light scattering methods.

Types of polymerization; kinetics of addition and step growth (condensation) polymerisation.

Different models for describing the size and shape of dissolved macromolecules; configuration and conformation of macromolecules. Diffusion and Stokes-Einstein equation.

Distribution of chain lengths: average end-to-end, root mean square end-to-end and most probable end-to-end chain length.

Recommended Books

1. Gupta, M. C., *Statistical thermodynamics*, New Age International Publishers, New Delhi (2007).
2. Levine, I. N., *Physical Chemistry*, 6^{th} Ed. McGraw Hill Education, New Delhi (2011).
3. Laidler, K. J., *Chemical Kinetics*, 3^{rd} Ed., Pearson Education, New Delhi (2011).
4. Kapoor, K. L., *A Textbook of Physical Chemistry: States of Matter and Ions in Solution*, Vol. I, 6^{th} Ed., McGraw Hill Education India (2019).
5. Kapoor, K. L., *A Textbook of Physical Chemistry: Thermodynamics and Chemical Equilibrium*, Vol. II, 6^{th} Ed., McGraw Hill Education India (2019).
6. Bockris, J. O. M.; Reddy, A. K. N., *Modern Electrochemistry 1: Ionics*, 2^{nd} Ed., Springer India, New Delhi (2018).
7. Bockris, J. O. M.; Reddy, A. K. N.; Gamboa-Aldeco, M., *Modern Electrochemistry 2A: Fundamentals of Electrodics*, 2^{nd} Ed., Vol. 2, Springer India, New Delhi (2006).
8. Billmeyer, F. W., *Textbook of Polymer Science*, 3^{rd} Ed., Wiley India, New Delhi (2007).

Further Reading

1. Puri, B. R.; Sharma, L. R.; Pathania, M. S., *Principles of Physical Chemistry*; 47^{th} Ed, Vishal Publishing, New Delhi (2017).
2. McQuarrie, D. A., *Statistical Mechanics*, Viva Books, New Delhi (2003).
3. Atkins, P. W.; de Paula, J.; Keeler, J., *Physical Chemistry*, 11^{th} Ed., Oxford University Press, New Delhi (2018).
4. Glasstone, S., *An Introduction to Electrochemistry*, Nabu Press, India (2011).
5. Gowariker, V. R., Viswanathan, N. V. and Sreedhar, J., *Polymer Science*, 3^{rd} Ed., New Age International Publishers, New Delhi (2019).
6. Moudgil, H. K., *Textbook of Physical Chemistry*, PHI Learning, New Delhi (2010).

SEMESTER II

CHEC 409 Molecular Spectroscopy

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: In this course on molecular spectroscopy, students will be introduced to the fundamental aspects of spectroscopy with special emphasis on the rotational, vibrational, Raman and electronic spectroscopies. Students will also be introduced to fundamental and application aspects mass spectrometry.

Learning outcome: Students will be able to understand and explain the theoretical basis of different spectroscopic techniques.

UNIT I: Rotational and Raman Spectroscopy

Rotational spectra of diatomic and polyatomic molecules. Intensities of rotational spectral lines, effect of isotopic substitution. Non-rigid rotators.

Classical theory of the Raman effect, polarizability as a tensor, polarizability ellipsoids, quantum theory of the Raman effect, Pure rotational Raman spectra of linear and asymmetric top molecules, Stokes and anti-Stokes lines.

Vibrational Raman spectra, Raman activity of vibrations, rule of mutual exclusion, rotational fine structure-O and S branches, Polarization of Raman scattered photons

UNIT II: Vibrational Spectroscopy

Vibrations of molecules, harmonic and anharmonic oscillators- vibrational energy expression, energy level diagram, vibrational wave functions and their symmetry, selection rules, expression for the energies of spectral lines, computation of intensities, hot bands, effect of isotopic substitution.

Diatomic vibrating rotor, vibrational-rotational spectra of diatomic molecules, P, R branches, breakdown of the Born-Oppenheimer approximation.

Vibrations of polyatomic molecules – symmetry properties, overtone and combination frequencies. Influence of rotation on vibrational spectra of polyatomic molecule, P, Q, R branches, parallel and perpendicular vibrations of linear and symmetric top molecules.

UNIT III: Electronic spectroscopy

Electronic Spectroscopy: Electronic spectroscopy of diatomic molecules, Frank-Condon principle, dissociation and predissociation spectra. $\pi\rightarrow\pi^*$, $n\rightarrow\pi^*$ transitions and their selection rules.

Photoelectron Spectroscopy: Basic principles, photoelectron spectra of simple molecules, X-ray photoelectron spectroscopy (XPS). Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems.

UNIT IV: Mass Spectrometry

Basic principle and instrumentation. Ionization techniques- Electron ionization (EI), chemical ionization (CI), desorption ionization (FAB/MALDI), electrospray ionization (ESI), isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution. Effect of isotopes on the appearance of mass spectrum.

Recommended Books

1. Banwell C. N.; McCash, E. M., *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill, New Delhi (2017).
2. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India, New Delhi (2015).
3. Sathyanarayana, D. N. *Handbook of Molecular Spectroscopy*, 2nd Ed., IK International Publishing, New Delhi (2019).
4. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., *Spectrometric Identification of Organic Compounds*, 8th Ed., Wiley India, New Delhi (2015).
5. Kemp, W., *Organic Spectroscopy*, 3rd Ed., Macmillan Publishers India, New Delhi (2011).

Further Reading

1. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds, Part A: Theory and Applications in Inorganic Chemistry*, 6th Ed., Wiley-Blackwell, New York (2009).
2. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry*, 6th Ed., Wiley-Blackwell, New York (2009).
3. Gunther, H., *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Ed., Wiley India, New Delhi (2010).
4. Dyer, J. R., *Applications of Spectroscopy of Organic Compounds*, PHI Learning, New Delhi (2004).
5. Aruldhas, G., *Molecular Structure and Spectroscopy*, 2nd Ed., Prentice Hall India, New Delhi (2007).

SEMESTER II

CHEC 410 Organic Chemistry Laboratory

Contact Hours per week: 6
Credits: 6
Terminal Examination Duration: 8 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This core laboratory course in organic chemistry introduces students to common organic chemistry laboratory practices, techniques for carrying out and monitoring a synthesis & extraction of natural products, and quantitative estimation/characterization of organic compounds.

Learning outcome: From this course, the students will understand organic chemistry from experimental point of view enabling them to perform qualitative analysis of organic compounds and mixtures. Students will learn techniques to extract and isolate organic and natural products.

1. Qualitative separation of binary mixture by physico-chemical method and determination of the functional groups by spectroscopic methods.

2. Monitoring of reaction by TLC, synthesis and isolation of organic compounds, separation/purification via extraction, recrystallization, distillation, basic idea on the application of column chromatography.

3. TLC studies of natural extracts and isolation of natural products:
   (a) Caffeine from tea leaves
   (b) Nicotine from tobacco
   (c) β-Carotene from carrot
   (d) Lycopene from tomato
   (e) Euginol from cloves
   (f) Casein from milk
   (g) Any other extraction possible in the laboratory

Recommended Text Book

1. Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R., *Vogel's Textbook of Practical Organic Chemistry*, 5th Ed., Pearson Education India, New Delhi (2003).

Further Reading

1. Mann, F. G.; Saunders, B. C., *Practical Organic Chemistry*, 4th Ed., Pearson Education India, New Delhi (2009).
2. Clarke, H. T., *A Handbook of Organic Analysis: Qualitative and Quantitative*, 4th Ed., CBS Publishers, New Delhi (2007).

SEMESTER III

CHEC 501 Materials Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course Objective: This course is aimed to introduce students to the interdisciplinary field of materials chemistry and nanomaterials, their synthetic and characterization techniques, properties and applications.

Learning outcome: Students will be able to examine/differentiate between different materials, and design/plan novel materials for applications.

UNIT II: Synthetic Methods
High temperature methods; co-precipitation and precursor method, sol-gel method; combustion synthesis, intercalation/de-intercalation reactions; High pressure synthesis-hydrothermal and template synthesis; chemical vapour deposition (CVD).
Synthesis of nanoparticle semiconductors, nanowires and nanorods; Synthesis, structures and properties of C_{60} and related compounds; Synthesis, structures and applications of single walled (SWNTs), multi-walled (MWNTs) carbon nanotubes. Other synthetic methods of nanomaterials (micellar and template based methods).

UNIT II: Characterization Techniques
X-ray methods: Powder X-ray Diffraction (PXRD), structure determination from PXRD, single crystal X-ray diffraction.
Thermoanalytical methods: Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.
Electron microscopy: Principles and application of scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive analysis of X-rays (EDAX).
Optical spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICP-MS), ICP-AES (Atomic Emission Spectroscopy), ICP-OES (Optical Emission Spectroscopy), Atomic Force Microscopy (AFM).

UNIT III: Electrical, Magnetic and Optical Properties
Electrical properties: Band theory of solids-metals and their properties; semiconductors - extrinsic and intrinsic, Hall effect; thermoelectric effects (Thomson, Peltier and Seebeck); insulators-dielectric, ferroelectric, pyroelectric and piezoelectric properties; ionic conductors.
Magnetic properties: Cooperative magnetism: Dia-, para-, ferro-, ferri-, and antiferromagnetic types; soft and hard magnetic materials; magnetoresistance.
Optical properties: Construction and application of GaSe and ruby laser.

UNIT IV: Chemistry of Advanced Materials
Superconductors: Brief history of superconductors, Properties of superconductors-critical temperature, effect of magnetic field; BCS theory; Superconductivity in 1-2-3 materials.

Applications of superconducting materials. Organic superconductors, Fullerenes and doped fullerenes as superconductors.
Intercalation compounds of graphite, Polymer-clay nanocomposites, Carbon-Carbon and polymer composite. Surface modification of nanomaterials with specific example to metal and metal oxide nanoparticles and their application in drug delivery, sensors, biosensors, catalysis, and in energy sector.

Recommended Books

1. West, A. R., *Solid State Chemistry and its Application*, Wiley India, New Delhi (2007).
2. Smart, L. E.; Moore, E. A., *Solid State Chemistry: An Introduction*, 4th Ed., CRC Press, New Delhi (2017).
3. Kakani, S. L.; Kakani, A., *Material Science*, 3rd Ed., New Age International Publishers, New Delhi (2016).
4. Skoog, D. A.; Holler, F. J.; Crouch, S. R., *Principles of Instrumental Analysis*, 6th Ed., Cengage Learning India, New Delhi (2014).
5. Willard, H. H.; Merritt, L. L.; Dean, J. A.; Settle, F. A., *Instrumental Methods of Analysis*, 7th Ed., CBS Publisher, New Delhi (2007).
6. Drago, R. S., *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing, Florida (1999).
7. Poole, C. P. Jr.; Owens, F. J., *Introduction to Nanotechnology*, Wiley India, New Delhi (2007).
8. Pradeep, T., *Nano: The Essentials-Understanding Nanoscience & Nanotechnology*, Tata McGraw Hill India, New Delhi (2017).

Further Reading

1. Rao, C. N. R.; Gopalakrishnan, J., *New Direction in Solid State Chemistry*, 2nd Ed., Cambridge University Press, Cambridge (1997).
2. Keer, H. V., *Principles of the Solid State*, 2nd Ed., New Age International Publishers, New Delhi (2017).
3. Braun, R. D.; *Introduction to Instrumental Analysis*, 2nd Ed., BSP Books, Hyderabad (2012).
4. Hornyak, G. L.; Tibbals, H. F.; Dutta, J.; Moore, J. J., *Introduction to Nanoscience and Nanotechnology*, CRC Press, Boca Raton (2008).
5. Viswanathan, B., *Nanomaterials*, Narosa Publishing House, New Delhi (2014).

SEMESTER III

CHEC 502 Applications of Molecular Spectroscopy

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course Objective: This course on spectroscopy, aimed at introducing students to the fundamental principles of magnetic resonance spectroscopy – NMR and ESR. Students will learn to solve composite problems using UV, IR, NMR and mass spectrometry in organic, inorganic and organometallic compounds.

Learning outcome: Students will be able to apply the principles of magnetic resonance and other spectroscopic techniques in elucidation of organic, inorganic and organometallic compounds.

UNIT I: NMR Spectroscopy

Basic principles: Zeeman effect, Magnetic properties of nuclei-Resonance condition, Nuclear spin, population of nuclear spin levels and NMR isotopes, relaxation methods. Instrumentation and sample handling; Classical approach and FT-NMR.
Chemical shift, Factors influencing chemical shifts: electronegativity and electrostatic effects; Mechanism of shielding and deshielding.
Spin systems: First order and second order coupling of AB systems, Simplification of complex spectra. Spin-spin interactions: Homonuclear coupling interactions - AX, AX_2, AX_3, AMX, AB types. Vicinal, germinal and long range coupling-spin decoupling. Nuclear Overhauser effect (NOE), Factors influencing coupling constants and Relative intensities.
^{13}CNMR, DEPT and structural correlations, Satellites. Brief introduction to 2D NMR – COSY, NOESY. Introduction to ^{31}P, ^{19}F NMR.

UNIT II: ESR spectroscopy

Characteristic features of ESR spectra, line shapes and line widths; ESR spectrometer. The *g* value and the hyperfine coupling parameter (*A*), origin of hyperfine interaction. Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy; Spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals. ESR spectra of magnetically dilute samples.

UNIT III: Application of Spectroscopic Techniques in Organic Chemistry

IR spectroscopy: Characteristic vibrational frequency/bands of hydrocarbons and important functional groups. Effects of H-bonding and solvents. Effects of unsaturation, substituents and ring size on vibrational frequencies of functional groups.
UV-Vis spectroscopy: λ_{max} and molar absorptivity, factors affecting them. Calculation of λ_{max} Woodward Fieser rule.
NMR: Applications of ^{1}H NMR and ^{13}C NMR in organic molecules.
Composite problems: Application of UV, IR, NMR and mass spectrometry in the structural elucidation of organic compounds.

UNIT IV: Application of Spectroscopic Techniques in Inorganic and Organometallic Chemistry

IR and Raman spectroscopy: Symmetry and IR/Raman activity of normal modes of vibration; mutual exclusion principle; interpretation of IR and Raman spectra of simple inorganic and coordination compounds. Vibrational spectra of metal carbonyls, metal carbonyl hydrides.

NMR Spectroscopy: Proton NMR spectra of metal hydride complexes, NMR spectra of nuclei other than hydrogen: ^{19}F, ^{31}P, ^{11}B NMR spectra of simple inorganic and organometallic compounds.

Composite problems: Application of UV, IR, NMR and mass spectrometry in the structural elucidation of organic compounds.

Recommended Books

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India, New Delhi (2015).
2. Sathyanarayana, D. N. *Handbook of Molecular Spectroscopy*, 2nd Ed., IK International Publishing, New Delhi (2019).
3. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., *Spectrometric Identification of Organic Compounds*, 8th Ed., Wiley India, New Delhi (2015).
4. Kemp, W., *Organic Spectroscopy*, 3rd Ed., Macmillan Publishers India, New Delhi (2011).

Further Reading

1. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds, Part A: Theory and Applications in Inorganic Chemistry*, 6th Ed., Wiley-Blackwell, New York (2009).
2. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry*, 6th Ed., Wiley-Blackwell, New York (2009).
3. Gunther, H., *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Ed., Wiley India, New Delhi (2010).
4. Dyer, J. R., *Applications of Spectroscopy of Organic Compounds*, PHI Learning, New Delhi (2004).
5. Drago, R. S., *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing (1999).
6. Figgis, B. N.; Hitchman, M. A., *Introduction to Ligand Field Theory and Its Applications*, Wiley India, New Delhi (2010).

SEMESTER III

CHEC 503 Organometallic & Heterocyclic Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course is intended for students to gain understanding about the organometallic compounds/reagents, their application in organic synthesis and catalysis. This course will also introduce students to heterocyclic chemistry.

Learning outcome: Students will be able to discuss/explain the synthesis, structure, & reactivity of organometallic compounds, reagents, demonstrate/plan their use in industrially important reactions.

UNIT I: Reactions of Organometallic Compounds

Substitution reactions-nucleophilic ligand substitution, nucleophilic and electrophilic attack on coordinated ligands.
Addition and elimination reactions-1,2 additions to double bonds, carbonylation and decarbonylation, oxidative addition and reductive elimination, insertion (migration) and elimination reactions.
Rearrangement reactions, redistribution reactions, fluxional isomerism.

UNIT II: Organometallic Compounds containing M-C, M=C and M≡C Bonds

Types of M-C bonds, synthesis and reactivity of metal alkyls, carbenes, alkenes, alkynes, and arene complexes; metallocenes and bent metallocenes.
Metal carbene complexes: Fischer, Schrock and Grubbs type carbene complexes, comparison of their stability and reactivity, reactions of Fischer carbene complexes and their synthetic utility; Alkene metathesis reactions using Schrock and Grubbs carbene metal complexes. Introduction to N-heterocyclic carbene metal complexes.
Metal carbyne complexes: synthesis, structure and reactivity

UNIT III: Catalysis by Organometallic Compounds

Homogeneous organometallic catalysis: alkene hydrogenation using Wilkinson catalyst; hydroformylation of olefins using cobalt or rhodium catalyst; Monsanto acetic acid process; oxidation of olefins by Wacker method; olefin oligomerization and isomerization. Palladium catalyzed C-C coupling reactions: Negishi, Suzuki, Stille, Heck and Sonogashira coupling
Heterogeneous organometallic catalysis: Fischer-Tropsch reaction, Ziegler Natta olefin polymerization.

UNIT IV: Heterocyclic Chemistry

Small Ring Heterocycles: Syntheses of aziranes, oxiranes & thiiranes; ring openings and heteroatom extrusion; synthesis & reactions of azetidines, oxetanes & thietanes.
Aromatic heterocycles: Synthesis and reactions of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole. Concept of π-excessive and π-deficient heterocyclics.

Condensed Five-membered Rings (1 Heteroatom): Synthesis and reactions of indole, benzofuran and benzothiophene.
Diazines: Structural & chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines, nucleophilic and electrophilic substitutions.

Recommended Books

1. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 5th Ed., Pearson Education, Essex (2018).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 6th Ed., Oxford University Press, New Delhi (2015).
3. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education India, New Delhi (2008).
4. Spessard, G. O.; Miessler, G. L., *Organometallic Chemistry*, 3rd Ed., Oxford University Press, Oxford (2015).
5. Elschenbroich, C., Organometallics, 3rd Ed., Wiley-VCH, Weinheim (2016).
6. Elias, A.; Gupta, B. D., *Basic Organometallic Chemistry: Concepts, Syntheses and Applications*, 2nd Ed., Universities Press, Hyderabad (2013).

Further Reading

1. Crabtree, R. H., *The Organometallic Chemistry of the Transition Metals*, 6th Ed., Wiley-Blackwell, New York (2014).
2. Acheson, R. M., *An Introduction to the Chemistry of Heterocyclic Chemistry*, 3rd Ed., Wiley India, New Delhi (2008).

SEMESTER III

CHEC 504 Inorganic Chemistry Laboratory

Contact Hours per week: 6
Credits: 6
Terminal Examination Duration: 8 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This core laboratory course in inorganic chemistry would expose students to experimental skills of qualitative and quantitative analysis and synthesis of coordination compounds with selected examples. Spectroscopic techniques like UV-visible, infrared, fluorescence etc. and other characterization techniques such as magnetic susceptibility and electrical conductivity measurements will be introduced.

Learning outcome: From this course, the students will be able to perfect experimental skills encompassing synthesis, characterization of different inorganic compounds. Students will learn to use instruments like UV-visible and FT-Infrared, fluorescence spectrophotometer through hand-on training.

1. Preparation and characterization by chemical analysis, IR and electronic spectrophotometry, magnetic susceptibility measurement, conductivity measurement, wherever appropriate and possible:
   (a) Preparation of Bis(acetylacetonate)oxovanadium, $VO(acac)_2$ and Oxidation of Anthracene by Hydrogen Peroxide in the Presence of $VO(acac)_2$.
   (b) Preparation of *Cis*-, *Trans*-Copper(II) glycine complexes.
   (c) Synthesis of Schiff base ligand, *bis*-(N, N'-disalicylalethylenediamine) and its Cobalt(II) complex.
   (d) Preparation of diethyldithiocarbamate and Nitrosylbis(diethyldithiocarbamato)iron, $Fe(NO)(S_2CNEt_2)_2$.
   (e) Estimation of Nickel as Bis(dimethyglyoximato)nickel(II), $Ni(dmg)_2$ by gravimetric method.
   (f) Estimation of Cobalt as mercury cobalt(II)tetrathiocyanate, $Hg[Co(SCN)_4]$ by gravimetric method.
   (g) Preparation of Werner complex, $[Co(NH_3)_5Cl]Cl_2$ and subsequent preparation of linkage isomers – $[Co(NH_3)_5NO_2]Cl_2$ and $[Co(NH_3)_5ONO]Cl_2$.

2. (a) Separation and determination of two metals: Ni-Zn, Cu-Fe, Ca-Mg, etc. involving volumetric and gravimetric methods.
   (b) Analysis of ores/alloys:
   Ores: Hematite, Limestone, Dolomite, Pyrolusite etc.
   Alloys: Brass, Gun metal, Cupro-nickel, Solder, Bronze, Phosphor-bronze.

Recommended Books

1. Mendham, J.; Denney, R. C.; Barnes, J. D.; Thomas, M.; Sivasankar, B., *Vogel's Textbook of Quantitative Chemical Analysis*, 6th Ed., Pearson Education, New Delhi (2009).
2. Raj, G., *Advanced Practical Inorganic Chemistry*, Krishna Prakashan, Meerut (2013).

SEMESTER III

CHEO 541 OPEN ELECTIVE: Environmental and Green Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course on environmental and green chemistry will educate the students about the concerns, remediation and perspective about environment and the global concerns. Students are expected to understand different aspects of environmental chemistry, chemistry of atmosphere, soil and water and fundamental aspects of green chemistry.

Learning Outcome: Students will be able to demonstrate an understanding of environmental chemistry, viz. air, water and soil pollution and their relationships vis-a-vis environment. Students will also learn green and sustainable methods developed in chemistry.

UNIT I: Atmospheric Chemistry
Temperature and pressure variation in the atmosphere, role of free radicals in atmospheric chemistry. Catalytic processes of ozone destruction, formation of Antarctic and Arctic ozone holes. Chemistry of smog formation, VOCs and their oxidation. Acid rain. PAHs and heavy metals in aerosols, lifetime and transport of aerosol particle. Global warming and greenhouse effect, Climate change Protocols. Sources of Indoor air pollution

UNIT II: Water and Soil Pollution
Sources of water pollution: agricultural and pesticidal pollutants, industrial and domestic effluent. Marine pollution, oil spills and oil pollution. Community wastewater treatment chemistry, biological process for removal of phosphorus and nitrogen from wastewater sources. Soil formation: Physical and Chemical weathering, Soil properties: Soil Texture, Cation exchange capacity, Causes of soil pollution, Chemistry and management of municipal and biomedical waste.

UNIT III: Environmental Toxicology and Detoxification Mechanism
Organic biocides, chemical stability, photolytic and non-photolytic reactions, hydrolysis, oxidation and reduction reactions, rates of degradative reactions, mobility of biocides. Principles of toxicology, chemical solution to environmental problems, better biodegradability. Kinetics of decomposition, solid remediation, chemical remediation and bioremediation.

UNIT IV: Principles of Green Chemistry
Principles of green chemistry, use of green starting materials and renewable feedstock, green solvents, green catalyst, less hazardous products, design for energy efficiency, design for degradation and real time analysis for pollution prevention.

Recommended Books

1. VanLoon G. W.; Duffey S. J., *Environmental Chemistry: A Global Perspective*, 4th Ed., Oxford University Press, Oxford (2017).
2. Anastas, P. T.; Warner, J. C., *Green Chemistry: Theory and Practice*, Oxford University Press, Oxford (2005).

Further Reading

1. Clark, J. H.; McQuarrie, D., *Handbook of Green Chemistry and Technology*, Wiley-Blackwell Publishing, Oxford (2002).
2. Pani, B., *A Textbook of Environmental Chemistry*, IK International Publishing House, New Delhi (2007).
3. Ahluwalia, V. K.; Kidwai M., *New Trends in Green Chemistry*, Springer Inida, New Delhi (2012).
4. Biswas, T. D.; Mukherjee, S. K. *Text Book of Soil Science*, Tata McGraw Hill India, New Delhi (2017).

SEMESTER III

CHEO 542 OPEN ELECTIVE: Bioanalytical and Medicinal Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course aims to introduce students to various types of drugs and medicines, sources of natural products and their chemistry, mode of action and theoretical aspects of drug design and action. Fundamental aspects, sampling techniques of Spectroscopic and analytical techniques will also be introduced.

Learning outcome: Through this course, students will be able to identify, describe and explain various aspects related to natural products derived from plants, animals, microbes and marine animals, drug design, drug action and structure-activity relationships.

UNIT I: Bioenergetics

The First law of thermodynamics, internal energy and enthalpy and relation between them. Enthalpies of formation, combustion, neutralization. The limitations of the first law of thermodynamics. Spontaneous process, Statement of second law. Concept of entropy, entropy change in reversible and irreversible processes. Free energy functions-criteria of spontaneity.
Redox reactions: oxidation number, balancing redox reaction, electrode potential, electrochemical series. Free energy change in redox reactions.

UNIT II: Spectroscopic and Analytical Techniques

Preparing samples for analysis: Classification of separation techniques, distillation, sublimation, recrystallization, precipitation, ion exchange, electrodeposition, volatilization, extraction chromatography. Introduction to high performance thin layer chromatography (HPTLC), high performance liquid chromatography (HPLC) and gas chromatography (GC).
Overview of spectroscopic techniques: basic idea and sampling techniques of atomic absorption/emission spectroscopy, IR, NMR (^{1}H, ^{13}C, ^{19}P, ^{14}N), UV and mass spectroscopy. Elemental analyses, X-Ray diffraction and X-Ray crystallography.

UNIT III: Medicinal Chemistry

Concept and definition of Pharmacophore. Pharmacodynamics and Pharmacokinetics.
ADMET of drugs: Factors affecting Absorption, Distribution, Metabolism, Elimination and Toxicity.
Drug Discovery, Design and Development. Structure activity relationships: Strategies in drug design. QSAR and combinatorial synthesis. Optimization of drug target interactions and access to drug targets. Pro-drugs and drug delivery systems. Brief idea about preclinical and clinical trials. Herbal drugs and their importance.

UNIT IV: Natural products in Drug Discovery

Introduction, sources (Plant, animal, microbial, marine), classification on chemical basis. Role of natural products in development of medicinal chemistry, providing “leads”.

Authentication and preparation of plant material/marine organisms. Screening of bioactive metabolites.
Extraction of Phytochemicals: Concepts of extraction with respect to activity guided fractionation and isolation of Markers/Biomarkers.
Natural products as medicinal agents along with their structurally modified form-Artemisinin, Ephedrines, Ergot alkaloids, Vasicine, Taxol.

Recommended Books

1. Atkins, P. W.; de Paula, J.; Keeler, J., *Physical Chemistry*, 11th Ed., Oxford University Press, New Delhi (2018).
2. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India, New Delhi (2015).
3. Sathyanarayana, D. N. *Handbook of Molecular Spectroscopy*, 2nd Ed., IK International Publishing, New Delhi (2019).
4. Harvey, D., *Modern Analytical Chemistry*, McGraw-Hill Higher Education (2000).
5. Lemke, T. L.; Zito, S. W.; Roche, V. F.; Williams, D. A., Essentials of *Foye's Principles of Medicinal Chemistry*. Wolters Kluwer India, New Delhi (2016).

Further Reading

1. Patrick, G. L., *An Introduction to Medicinal Chemistry*. 5th Ed.; Oxford University Press, New Delhi (2013).
2. Silverman, R. B., *The Organic Chemistry of Drug Design and Drug Action*, 2nd Ed.; Elsevier Academic Press, Cambridge, Massachusetts (2012).

SEMESTER III

CHEO 543 OPEN ELECTIVE: Applications of Molecular Spectroscopy

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course Objective: This course on spectroscopy, aimed at introducing students to the fundamental principles of UV-Vis, IR, Raman, magnetic resonance spectroscopy – NMR and ESR, with emphasis on application. Students will also be introduce to modern methods characterization of advanced materials.

Learning outcome: Students will be able to apply the principles of magnetic resonance and other spectroscopic techniques in elucidation of organic, inorganic and organometallic compounds. Fundamental Knowledge about the modern methods of characterization techniques will help the students to examine and apply the techniques.

UNIT I: Application of UV-Visible, IR, NMR and Raman Spectroscopy

IR spectroscopy: Characteristic vibrational frequency/bands of hydrocarbons and important functional groups. Effects of H-bonding and solvents. Effects of unsaturation, substituents and ring size on vibrational frequencies of functional groups.

UV-Vis spectroscopy: λ_{max} and molar absorptivity, factors affecting them. Calculation of λ_{max} Woodward Fieser rule.

IR and Raman spectroscopy: Symmetry and IR/Raman activity of normal modes of vibration; mutual exclusion principle; interpretation of IR and Raman spectra of simple molecues.

NMR: Applications of ^{1}H NMR and ^{13}C NMR in organic molecules.

Composite problems: Application of UV, IR, NMR and mass spectrometry in the structural elucidation of organic compounds.

UNIT II: Magnetic Resonance Spectroscopy

NMR Spectroscopy: Structural elucidation of organic molecules-alcohols, aldehydes, ketones, amides, ester olefin etc. Simple applications to inorganic compounds and coordination compounds: ^{1}H, ^{13}C, ^{31}P, ^{19}F. NMR spectra of paramagnetic compounds.

ESR Spectroscopy: Interpretation of ESR spectra and structure elucidation of organic radicals using ESR spectroscopy; Spin-orbit coupling and significance of g-tensors, zero/non-zero field splitting, Kramer's degeneracy, application to transition metal complexes (having one to five unpaired electrons) including biological molecules and inorganic free radicals.

UNIT III: Mass Spectrometry

Basic principle and instrumentation. Ionization techniques- Electron ionization (EI), chemical ionization (CI), desorption ionization (FAB/MALDI), electrospray ionization (ESI), isotope abundance, molecular ion, fragmentation processes of organic molecules, deduction of structure through mass spectral fragmentation, high resolution. Effect of isotopes on the appearance of mass spectrum. Application to organometallic compounds.

UNIT IV: Modern Methods of Characterization Techniques

X-ray methods: Powder X-Ray Diffraction (PXRD), structure determination from PXRD, X-ray photoelectron spectroscopy.

Thermoanalytical methods: Thermo gravimetric analysis, differential thermal analysis and differential scanning calorimetry.

Electron microscopy: Principles and application of scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive analysis of X-rays (EDAX).

Optical spectroscopy: Inductively coupled Plasma- mass spectroscopy (ICP-MS), ICP-AES (Atomic Emission Spectroscopy), AIP-OES (Optical Emission Spectroscopy)

Recommended Books

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 5th Ed., Cengage Learning India, New Delhi (2015).
2. Sathyanarayana, D. N. *Handbook of Molecular Spectroscopy*, 2nd Ed., IK International Publishing, New Delhi (2019).
3. Silverstein, R. M.; Webster, F. X.; Kiemle, D. J.; Bryce, D. L., *Spectrometric Identification of Organic Compounds*, 8th Ed., Wiley India, New Delhi (2015).
4. Kemp, W., *Organic Spectroscopy*, 3rd Ed., Macmillan Publishers India, New Delhi (2011).

Further Reading

1. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds, Part A: Theory and Applications in Inorganic Chemistry*, 6th Ed., Wiley-Blackwell, New York (2009).
2. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds, Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry*, 6th Ed., Wiley-Blackwell, New York (2009).
3. Gunther, H., *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Ed., Wiley India, New Delhi (2010).
4. Dyer, J. R., *Applications of Spectroscopy of Organic Compounds*, PHI Learning, New Delhi (2004).
5. Drago, R. S., *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing (1999).
6. Figgis, B. N.; Hitchman, M. A., *Introduction to Ligand Field Theory and Its Applications*, Wiley India, New Delhi (2010).

SEMESTER IV

CHEC 505 Biochemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course is intended to introduce the students to different biochemical systems involved in the life processes.

Learning outcome: Students will be able to appreciate, describe and interpret the chemical and physical processes of living organisms.

UNIT I: Cell Structure and Metabolic Processes

Cell structure: Prokaryotic and eukaryotic cells; Intracellular organelles and their functions; Comparison of plant and animal cells. Origin of life- unique properties of carbon, chemical evolution and rise of living system.

Metabolic processes: Catabolism and anabolism, ATP- currency of biological energy, energy rich and energy poor phosphates, biological redox agents.

UNIT II: Enzymes and Proteins

Introduction, classification and characteristics of enzymes. Salient features of active site of enzymes. Mechanism of enzyme action (taking chymotrypsin as example), factors affecting enzyme action, coenzymes and cofactors and their role in biological reactions, specificity of enzyme action (including stereospecificity), enzyme inhibitors and their importance, phenomenon of inhibition (competitive, uncompetitive and non-competitive inhibition including allosteric inhibition). Protein conformations– globular and fibrous. Ramachandran plot. Protein folding and denaturation.

UNIT III: Lipids and Nucleic Acids

Definition, nature, biological importance of fatty acids and lipids, saturated and unsaturated fats, ketone bodies, fatty acid metabolism, calorific value of foods. Triglycerides, phospholipids, glycolipids, steroids. Brief introduction to biological membranes, properties and function of lipid bilayers and liposomes.

Nucleotides and nucleosides, structure of nucleic acids, Chemical and enzymatic hydrolysis of nucleic acids, purine metabolism, DNA Replication, Types of RNA. Role of DNA and RNA (m-RNA, t-RNA, r-RNA) in protein biosynthesis. Genetic code and basis of hereditary. Gene mutation and carcinogenesis.

UNIT IV: Metabolic processes

Glycolysis, fate of pyruvate under anaerobic condition, TCA cycle and gluconeogenesis. Electron transport and oxidative phosphorylation. Photosynthesis-light and dark reactions.

Recommended Books

1. Berg, J. M.; Tymoczko, J. L.; Gatto Jr., G. J.; Stryer, L., *Biochemistry*, 9^{th} Ed., W. H. Freeman, New York (2019).
2. Voet, D.; Voet, J. G., Pratt, C. W., *Biochemistry*, 4^{th} Ed., John Wiley and Sons, New Jersey (2012).

Further Reading

1. Campbell, M. K.; Farrell, S. O., *Biochemistry*, 8^{th} Ed., Brooks/Cole, Belmont (2015).
2. Nelson, D. L.; Cox, M. M., *Lehninger Principles of Biochemistry*, 7^{th} Ed., W. H. Freeman, New York (2017).

SEMESTER IV

CHEE 511 ELECTIVE I: Inorganic Reaction Mechanisms

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course will expose the students to the concepts of inorganic reaction mechanisms and inorganic photochemistry.

Learning outcome: Students will be able to apply their knowledge of inorganic reaction mechanism to interpret and critically examine the reactivity of metal complexes.

UNIT I: Ligand Substitution Reactions
Ligand Substitution Reactions: Inter and Labile Complexes; Mechanisms of Substitution reaction and their kinetic consequences. Ligand substitution reactions in octahedral complexes: ligand and steric effect on reaction rate; water exchange, The Eigen-Wilkins mechanism; base catalyzed hydrolysis; isomerization and racemization reactions. Ligand substitution in square planar complexes: trans effect and its influence.

UNIT II: Redox Reactions
Inner sphere electron transfer, Taube mechanism, bridging ligand effect; outer sphere electron transfer, Marcus theory, Excited state outer sphere electron transfer reactions, use of electron transfer reactions for the synthesis of complexes.
Half cell reaction, redox potential, electrochemical series, Nernst equation, Latimer and Frost diagram, disproportionation reactions, basics of cyclic voltammetry.

UNIT III: Photochemical Reactions
Introduction to Inorganic Photochemistry, photophysical and photochemical processes, characteristics of the electronically excited states of inorganic compounds–ligand field states, charge transfer states, Frank-Condon, and thexi states, kinetics of photochemical process. Photochemical reactions: substitution and redox reactions of chromium, cobalt and ruthenium complexes. Relevance of ruthenium polypyridine complexes in solar energy conversion and storage, photo splitting of water, Inorganic photochemistry in biological processes and their model studies.

UNIT IV: Metal-Metal Bond and Clusters
Definition of metal clusters, metal-metal multiple bonding in $[M_2X_8]^{2-}$, metal halide clusters. Metal-carbonyl clusters – Low Nuclearity Carbonyl Clusters (LNCC) and High Nuclearity Carbonyl Clusters (HNCC), Clusters having interstitial main group elements. Polyhedral Skeletal Electron Pair Theory (PSEPT), capping rules, isolobal relationships between main-group and transition metal fragments. Molecular clusters in catalysis.

Recommended Books

1. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 5th Ed., Pearson Education, Essex (2018).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 6th Ed., Oxford University Press, New Delhi (2015).
3. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education India, New Delhi (2008).
4. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education India, New Delhi (2006).

Further Reading

1. Jordan, R. B.; *Reaction Mechanisms of Inorganic and Organometallic Systems*, 3rd Ed., Oxford University Press, New York (2007).
2. Roundhill, D. M., *Photochemistry and Photophysics of Metal Complexes*, Plenum: New York (1994).
3. Basolo, F.; Pearson, R. G., *Mechanisms of Inorganic Reactions: Study of Metal Complexes in Solution*, 2nd Ed., John Wiley and Sons, New Jersey (1975).

SEMESTER IV

CHEE 512 ELECTIVE II: Bioinorganic Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course introduces students to the advanced knowledge of role of metal ions in biological systems and their structure function relationship..

Learning outcome: Students will learn the role of metal ions in biological systems, toxicity due to metal ions, the role in diseases and therapy.

UNIT I: Bioinorganic Chemistry

Scope, inorganic elements in biological system. Mechanism of ion transport across membrane: Energetics of transport, kinetics and mechanism of transport, ionophores, valinomycin; ATP mediated active transport, Na^+/K^+ pump. Ca^{2+} transport. Role of calcium in muscle contraction, blood-clotting mechanism.

Photosynthesis: Chlorophyll-structural features, role of Mg^{2+}, Z-scheme of photosynthesis-PSI and PSII. Water Oxidation Centre (WOC) and model studies.

UNIT II: Iron-Containing Proteins and Enzyme

Oxygen transport and oxygen uptake proteins: transport and storage of dioxygen; Heme proteins and oxygen uptake, structure and functions of hemoglobin and myoglobin, dioxygen binding, cooperativity effect, Bohr effect, Hill equation; Model complexes for dioxygen binding; Non-heme systems: hemerythrin and hemocyanin. Cytochromes: cytochrome *c*, cytochrome P-450. Iron sulfur proteins: rubredoxin and ferredoxin. Iron enzymes: peroxidase, catalase. Iron storage and transport: siderophores, ferritin and transferrins.

UNIT III: Mo, Cu, Zn and Co-Containing Enzymes

Molybdenum-containing enzyme: xanthine oxidase; nitrate reductase, nitrogenase, Biological fixation of N_2.

Copper containing enzymes: superoxide dismutase, cytochrome c oxidase, plastocyanin and ceruloplasmin.

Zinc-containing enzymes: zinc fingers, carbonic anhydrase, carboxypeptidase, alcohol dehydrogenase, phosphodiesterase and nuclease, interchangeability of zinc and cobalt in enzymes.

Cobalt-containing enzymes: Vitamin B_{12} and B_{12} coenzymes and cyanocobalamin.

UNIT IV: Metals in Medicine

Metal deficiency and disease; toxicity of mercury, cadmium, lead, beryllium, selenium and arsenic; biological defence mechanisms; chelation therapy; metals used for diagnosis and chemotherapy, platinum complexes as anticancer drugs, Pt-DNA binding, complexes of gold, copper, zinc, mercury, arsenic and antimony as drugs.

Recommended Books

1. Kaim, W.; Schwederski, B.; Klein, A., *Bioinorganic Chemistry-Inorganic Elements in the Chemistry of Life: An Introduction and Guide*, 2nd Ed., John Wiley & Sons, West Sussex (2013).
2. Bertini, I.; Gray, H. B.; Lippard, S. J.; Valentine, J. S., *Bioinorganic Chemistry*, Viva Books, New Delhi (2007).
3. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 5th Ed., Pearson Education, Essex (2018).
4. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 6th Ed., Oxford University Press, New Delhi (2015).
5. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education India, New Delhi (2006).

Further Reading

1. Rehder, D., *Bioinorganic Chemistry*, Oxford University Press, London (2014)
2. Roat-Malone, R. M., *Bioinorganic Chemistry: A Short Course*, 2nd Ed., Wiley-Blackwell, New York (2007).
3. Reddy, K. H., *Bioinorganic Chemistry*, New Age International Publishing, New Delhi (2009).

SEMESTER IV

CHEE 513 ELECTIVE III Advanced Inorganic Chemistry Laboratory

Contact Hours per week: 12
Credits: 12
Terminal Examination Duration: 8 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This advanced laboratory course on inorganic chemistry would expose students to experimental skills of advanced material synthesis, characterization and study of their properties with selected examples. Spectrophotometric techniques and green chemistry experiments will also be introduced.
Students will also learn to survey research literature, and collect/compile the information for preparing reports and for publications.

Learning outcome: From this course, students will be able to perfect experimental skills encompassing synthesis, characterization of advanced materials. Students will learn to use instruments like UV-visible and FT-Infrared, fluorescence spectrophotometer through hand-on training for analysis, data collection and interpretation.

Advanced Practical (6 Credit)

1. Preparation of:
   (a) Synthesis of metal acetylacetonate complexes using green chemistry approach.
   (b) Synthesis of metal nanoparticles (Cu, Ag, Au, etc.), characterization and investigation of their optical properties.
   (c) Synthesis and characterization of semiconductor nanocrystals (CdS, ZnS, ZnO etc.).
   (d) Preparation of polyoxometallates (e.g. tetrabutylammoniumhexamolybdate(VI)) and characterization.

2. Spectrophotometry:
   (a) Spectrophotometric estimation of Fe, Ni, Co.
   (b) Determination of composition of binary mixtures by spectrophotometric method (e.g. $K_2Cr_2O_7$ and $KMnO_4$).

New innovative experiments may be introduced from time to time.

Literature Survey (6 Credit)
The student will undertake literature survey on a topic related to his/her specialization under the guidance of one faculty member. He/she will write a report and give a presentation at the time of end semester examination. The average of the marks given by the external and the internal examiners will be awarded to the student.

Recommended Books

1. Mendham, J.; Denney, R. C.; Barnes, J. D.; Thomas, M.; Sivasankar, B., *Vogel's Textbook of Quantitative Chemical Analysis*, 6th Ed., Pearson Education, New Delhi (2009).
2. Raj, G., *Advanced Practical Inorganic Chemistry*, Krishna Prakashan, Meerut (2013).
3. Sharma, R. K.; Sidhwani, I. T.; Chaudhari, M. K. *Green Chemistry Experiment: A Monograph*, I. K. International Publishing, New Delhi (2012).

SEMESTER IV

CHEE 521 ELECTIVE I: Organic Synthesis I

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This course will enable the students to comprehend the basics of retrosynthesis and its importance in planning an organic synthesis, important reagents and methods of organic synthesis.

Learning outcome: Through this course students will acquire the detailed knowledge on planning of synthesis of complex organic molecules and about reagents and methods to achieve targeted synthetic molecules.

UNIT I: Planning a Synthesis
Retrosynthesis, synthons and synthetic equivalents, disconnection approach, functional group inter-conversions, importance of order of events in organic synthesis.
One and two group C-X disconnection: synthesis of alcohols, ethers, sulfides, amines; chemoselectivity guidelines; One group C-C disconnections: in alcohols and carbonyl compounds, regioselectiviity, Two group C-C disconnections: Diels-Alder reaction, α,β -unsaturated carbonyl compounds, control in carbonyl condensations, difunctionalised compounds, Michael addition and Robinson annulation.

UNIT II: Advanced Topics in Stereochemistry
Conformations of fused polycyclic systems: decalin, 1-decalone and 2-decalone; Stereochemistry of C-C bond formations reactions involving enolate anions; ring size and ease of cyclisation reactions: Baldwin's rule.
Effect of conformation of reactivity of cyclohexane: Hydrolysis of esters of cyclohexane carboxylic acid, esterification of cyclohexane carboxylic acids, substitution and elimination in cyclohexane system, reduction of cyclohexanol, rearrangement involving cycohaxanes, epoxidation of cyclohexane halohydrin.

UNIT III: Reagents in Organic Synthesis
9-BBN, IBX, Dess-Martin periodinane, Fetizon reagent, dioxiranes, Gilman's reagent, lithium disopropylamide, dicyclohexylcarbodimide, 1,3-dithiane reactivity: Umpolung effect, Phase transfer catalyst, Tebbe reagent, Baker's yeast, NBS, Mosher's reagent, DDQ.

UNIT IV: Modern Synthetic Methods
Metal mediated C-N coupling reactions: Buchwald-Hartwig, Ullmann and Chan-Lam cross-coupling reactions; Olefination reactions: McMurry, Peterson and Julia olefination reactions; Biginelli reaction, Hantzsch reaction, Ugi reaction, Mitsonobu reaction, Nef reaction, Henry reaction.

Recommended Books

1. Warren, S., *Organic Synthesis: The Disconnection Approach*, Wiley India, New Delhi (2007).
2. Nasipuri, D. Stereochemistry of Organic Compounds: Principles and Applications, 3rd Ed., New Age International Publishers, New Delhi (2018).
3. Carruthers, W., *Modern Methods of Organic Synthesis*, 4th Ed., Cambridge University Press, New Delhi (2005).

Further Reading

1. Smith, M. B., *Organic Synthesis*, 4th Ed., Academic Press, Cambridge, Massachusetts (2016).
2. Kurti, L., Czako, B., *Strategic Application of Named Reactions in Organic Synthesis,* Elsevier, Amsterdam (2005)

SEMESTER IV

CHEE 522 ELECTIVE II: Natural Products and Medicinal Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: In this course, students will be introduced to various types of drugs and medicines, their chemistry, mode of action and theoretical aspects of drug design and action.

Learning outcome: Students will be able to identify, compare and explain aspects related to drug design, drug action and SARs.

UNIT I: Terpenoids and Alkaloids

Terpenoids: Definition, classification and structure determination (general methods), chemistry of some important terpenoids: geraniol, limonene, carvone.
Alkaloids: Introduction, isolation technique, general methods of structure determination, classification, chemistry of some well-known alkaloids: morphine, heroin, quinine, nicotine reserpine, etc.

UNIT II: Steroids

Introduction, sterols: constitution of cholesterol, bile acids: isolation, constitution and function; hormones: classification, biological significances, constitution of oestrone and androsterone.

UNIT III: Medicinal Chemistry

Concept and definition of pharmacophore, pharmacodynamics and pharmacokinetics.
Drug targets: enzymes and receptors, competitive, non-competitive and allosteric inhibitors, transition state analogues and suicide substrates. Nucleic acids as drug targets: reversible DNA binding agents, DNA alkylating agents and DNA strand breakers.

UNIT IV: Natural Products in Drug Discovery

Drug Discovery, design and development. ADMET of drugs: Factors affecting Absorption, Distribution, Metabolism, Elimination and Toxicity.
Structure-activity relationships: Strategies in drug design. QSAR and combinatorial synthesis. Optimization of drug target interactions and access to drug targets. Pro drugs and drug delivery systems.

Recommended Books

1. Finar, I. L. *Organic Chemistry*, 5th Ed., Vol. 2, Pearson Education, New Delhi (2011).
2. Patrick, G. L., *An Introduction to Medicinal Chemistry*. 5th Ed.; Oxford University Press, New Delhi (2013).
3. Silverman, R. B., *The Organic Chemistry of Drug Design and Drug Action*, 2nd Ed.; Elsevier Academic Press, Cambridge, Massachusetts (2012).

Further Reading

1. Mann, J.; Davidson, R. S.; Hobbs, J. B.; Banthrope, D. V., Harborne, J. B., *Natural Products, Their Chemistry and Biological Significance*, Longman, Essex (1994).
2. Lemke, T. L.; Zito, S. W.; Roche, V. F.; Williams, D. A., Essentials of *Foye's Principles of Medicinal Chemistry*. Wolters Kluwer India, New Delhi (2016).

SEMESTER IV

CHEE 523 ELECTIVE IV: Advanced Organic Chemistry Laboratory

Contact Hours per week: 12
Credits: 12
Terminal Examination Duration: 8 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This advanced laboratory course on organic chemistry would expose students to experimental skills of multistep organic synthesis through conventional and greener practice. Students will also learn to survey research literature, and collect/compile the information for preparing reports and for publications.

Learning outcome: From this course, the students will be able to perfect experimental skills of multistep synthesis of organic molecules.

Advanced Practical (6 Credit)

1. Organic preparations involving two or more steps:
   (a) Benzopinacolone from benzophenone via benzopinacol
   (b) Benzilic acid from benzoin
   (c) Dibenzyl from benzoin
   (d) Anthranilic acid from phthalic anhydride
   (e) Any halogenation reaction etc.

2. Greener practice in organic synthesis:
   (a) Acetylation of primary amine
   (b) Bromination of acetanilide
   (c) Nitration of phenol
   (d) Pinacol Pinacolone rearrangement
   (e) Any other possible reaction

New innovative experiments may be introduced from time to time.

Literature Survey (6 Credit)

The student will undertake literature survey on recent advances in chemistry related to his/her specialization under the guidance of one faculty member. He/she will write a report and give a presentation at the time of end semester examination. The average of the marks given by the external and the internal examiners will be awarded to the student.

Books Recommended

1. Furniss, B. S.; Hannaford, A. J.; Smith, P. W. G.; Tatchell, A. R., *Vogel's Textbook of Practical Organic Chemistry*, 5th Ed., Pearson Education, New Delhi (2005).
2. Sharma, R. K.; Sidhwani, I. T.; Chaudhari, M. K. *Green Chemistry Experiment: A Monograph*, I. K. International Publishing, New Delhi (2012).

SEMESTER IV

CHEE 531 ELECTIVE I: Polymer Chemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course Objective: Students will be introduced to the field of polymer chemistry, synthetic methods and characterization.

Learning outcome: Students will be able to use the understanding gained for the synthesis and characterization of polymer materials for designing novel polymeric materials for applications.

UNIT I: Introduction

Historical background, types, classification and importance of polymers, chemical and geometrical structure, physical state and thermal transition: crystalline melting temperature, T_m and glass transition temperature, T_g.
Properties of polymers: thermal, mechanical, rheological and electrical properties.
Applications and future trends of polymers

UNIT II: Polymerization Processes

Step polymerization, chain polymerization including carbonyl polymerization, ionic polymerization, co-ordination polymerization, atom transfer free radical polymerization, supramolecular polymerization, ring opening polymerization, metathesis polymerization, group transfer polymerization; emulsion polymerization, chain copolymerization. Reactivity ratio and control of molecular weight in polymerization.

UNIT III: Polymer Characterization

Average molecular weight concept, Number average, weight average, viscosity average molecular weights. Polydipersity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group analysis, viscosity, light scattering, osmotic and ultrantracentrifugation methods, fractionation of polymers, Gel permeation chromatography (GPC).
Chemical analysis of polymers: Spectroscopic methods, X-ray diffraction study, microscopy, thermal analysis.

UNIT IV: Thermodynamics of Polymer Solutions

Chain conformation, kinetic chain length; molecular dimensions in solution, solubility of polymers, solubility parameters, transfer process, lattice theory, thermodynamics of polymer dissolution; ΔH, ΔS and ΔG of mixing; Flory–Huggins theory, thermodynamics of dilute polymer solutions, χ_1 and θ-temperature.

Recommended Books

1. Sun, S. F., *Physical Chemistry of Macromolecules: Basic Principles and Issues*, 2nd Ed., Wiley-Blackwell, New York (2004).
2. Odian, G., *Principle of Polymerization*, 4th Ed., Wiley-Blackwell, New York (2004).
3. Flory, P. J., *Principles of Polymer Chemistry*, Asian Books, New Delhi (2006).
4. Gowariker, V. R.; Viswanathan, N. V.; Sreedhar, J., *Polymer Science*, New Age International Publishers, New Delhi (2011).

Further Reading

1. Misra, G. S., *Introduction to Polymer Chemistry*, New Age International Publishers (2008).
2. Billmeyer, F. W., *Textbook of Polymer Science*, Wiley India, New Delhi (2010).

SEMESTER IV

CHEE 532 ELECTIVE II: Advanced Chemical Kinetics and Photochemistry

Contact Hours per week: 4
Credits: 4
Terminal Examination Duration: 3 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This is course on physical chemistry covers advanced chemical kinetics focusing on reactions in solutions and reaction dynamics. This course will also cover photochemical aspects.

Learning outcome: This course will help the students to understand dynamics of chemical reactions and their implications.

UNIT I: Study of Chemical Reactions

Methods of studying chemical reactions: molecular beam study; stopped flow technique, temperature and pressure jump methods, NMR studies in fast reactions, shock tube kinetics. Relaxation kinetics: linearized rate equation, relaxation time in single step fast reactions, determination of relaxation time and rate constant.

UNIT II: Reactions in Solutions

Kinetics of ion – ion and ion – dipole reactions, effect of dielectric constant on reaction rate; effect of pressure on reaction rate; cage reactions, cluster reactions, electron transfer reactions, kinetics of diffusion controlled reactions; transport phenomena; Linear free energy relationship, Hammet equation, Taft equation and their applications.

UNIT III: Molecular Reaction Dynamics

Potential energy surfaces; features of potential energy surfaces; estimation of activation energy and calculation of potential energy surfaces; collisions of real molecules; trajectory calculations.

Dynamics of unimolecular reactions: limitations of Lindemann and Hinshelwood theory, RRK theory, RRKM theory (quantitative treatment). Femtochemistry: dynamics and chemical reactivity.

UNIT IV: Photochemistry

Laws of Photochemistry; absorbance of a solution; determination of equilibrium constant; primary and secondary processes; quantum efficiency.

Photophysical processes: types and radiationless transitions; photophysical kinetics: unimolecular and bimolecular processes; delayed fluorescence; fluorescence quenching and Stern–Volmer equation, concentration dependence of quenching and excimer formation, quenching by added substances. Electronic energy transfer mechanism of quenching, photosensitization.

Photochemical processes: types of photochemical processes; kinetics of photochemical reactions; photostationary state and quenching of fluorescence; photosensitized reactions; flash photolysis technique and fluorescence quenching technique.

Recommended Books

1. Laidler, K. J., *Chemical Kinetics*, 3rd Ed., Pearson Education, New Delhi (2011).
2. Rajaram, V.; Kuriakose, J. C., *Kinetics and Mechanism of Chemical Transformation*, McMillan India, New Delhi (2009).
3. Rohatgi-Mukherjee, K. K., *Fundamentals of Photochemistry*, 3rd Ed., New Age International Publishers, New Delhi (2013).

Further Reading

1. Pilling, M. J.; Pilling, S.; Seakins, P. W., *Reaction Kinetics*, Oxford University Press, London (1996).
2. Valeur, B., *Molecular Fluorescence: Principles and Applications*, Wiley-VCH, Weinheim (2002)
3. Ronda, C., *Luminesence: From Theory to Applications*, Wiley-VCH, Weinheim (2008).

SEMESTER IV

CHEE 533 ELECTIVE III: Advanced Physical Chemistry Laboratory

Contact Hours per week: 12
Credits: 12
Terminal Examination Duration: 8 Hours
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective: This advanced laboratory course on physical chemistry would expose students to the skills of performing and comprehending various physical chemistry experiments such as chemical kinetics, surface chemistry, thermodynamics, spectrophotometry etc..
Students will also learn to survey research literature, and collect/compile the information for preparing reports and for publications.

Learning outcome: From this course, the students will be able to perfect experimental skills from physical chemistry point of view.

Advanced Practical (6 Credit)

1. To study the kinetics of reaction between $K_2S_2O_8$ and KI and hence determine the rate constant and order of the reaction. Also study the influence of ionic strength on the reaction rate.
2. To determine the relative strengths of two acids by studying the acid catalysed hydrolysis of methyl acetate (use least square fitting).
3. To study the variation of surface tension of aqueous solution of *n*-propyl alcohol at different concentration and hence determine the limiting cross-sectional area of the alcohol molecule.
4. To compare the cleansing powers of two samples of detergent by surface tension method.
5. To determine critical solution temperature of phenol and water in presence of (a) 1% NaCl (b) 0.5% naphthalene and (c) 1% succinic acid.
6. To study the variation of solubility of $Ca(OH)_2$ in NaOH solution and hence determine its solubility product.
7. To determine the formula of the complex formed between the cupric ion and ammonia by distribution method.
8. To study the influence of ionic strength on the solubility of $CaSO_4$ and hence determine its thermodynamic solubility product.
9. To compare the relative strengths of acetic acid and monochloroacetic acid by conductometric method.
10. To determine the standard electrode potential of the ferrous/ferric system by potentiometric titration of ferrous ammonium sulphate against potassium dichromate.
11. To study the saponification of ethyl acetate by sodium hydroxide conductometrically and determine the order of reaction and activation energy.
12. To determine apparent ionization constant of acetic acid by potentiometric titration against NaOH solution.
13. Determine the dissociation constant of methyl red by spectrophotometric method.
14. To determine the composition of binary mixture containing $KMnO_4$ and $K_2Cr_2O_7$ spectrophotometrically.

15. To determine the dissociation constant of an indicator (e.g. methyl red) by spectrophotometric method.
16. To estimate the concentration of HCl, CH_3COOH and $CuSO_4$ in a mixture by conductometric titration.
17. To determine the partial molar volume of ethanol–water mixture at a given composition.

Literature Survey (6 Credit)

The student will undertake literature survey on a topic related to his/her specialization under the guidance of one faculty member. He/she will write a report and give a presentation at the time of end semester examination. The average of the marks given by the external and the internal examiners will be awarded to the student.

Recommended Books

1. Halpern, A. M.; McBane, G. C., *Experimental Physical Chemistry: A Laboratory Textbook*, W. H. Freeman, New York (2006).
2. Viswanathan, B.; Raghavan, P. S., *Practical Physical Chemistry*, Viva Books, New Delhi (2014).
3. Yadav, J. B., *Advanced Practical Physical Chemistry*, Krishna Prakashan, Meerut (2015).

SEMESTER IV

CHEE 551 ELECTIVE IV Project Dissertation

Contact Hours per week: 12
Credits: 12
Terminal Examination Duration: Oral Presentation
Maximum Marks: **100** (Terminal – 80, Sessional – 20)

Course objective:
The purpose of offering project work to the students is to encourage the students in research and innovation in frontier areas of chemistry. Through this course they would be introduced to various stages of research planning and implementation. Students will perform scientific research under the supervision of a faculty and learn to work independently.
During the course of her/his project work, students are expected to learn different synthetic methods and analytical techniques for carrying out scientific research problems, particularly to collect and interpret data.

Learning outcome:
Following the completion of this course, students should be able demonstrate ability to plan and strategize a scientific research problem, and implement it within a reasonable time frame. It is expected that after completing this project dissertation, students will learn to work independently and how to keep accurate/readable record of their experimental work.
In addition, students will be able to handle laboratory equipment and chemicals. Also, students will be able to utilize sophisticated instruments for analysis, data collection and interpretation.
Subsequently, the students should be able to critically examine research articles, and improve their scientific writing/communication skills.

Instructions:

- Project work would be in lieu of Advanced Inorganic Chemistry Laboratory and Literature Survey (CHEE 513/ CHEE 523/ CHEE 533).
- For project work, the area of the work would be to be decided by the advisor. On completion of the project work, students have to submit the work in the form of a dissertation followed by oral presentation in the presence of faculty members and external expert(s).