MSc Chemistry (CBCS) Syllabus

Department of Chemistry

Rajiv Gandhi University
Arunachal Pradesh

Contents

PREFACE

As per the directive from the Rajiv Gandhi University, the syllabus for the 2-year M.Sc. course in Chemistry was prepared. The University provided the guidelines for the Choice Based Credit System (CBCS).

Keeping in view the need to impart value based education; a student friendly syllabus incorporating new ideas and theories in frontier areas of chemistry has been prepared. Focus has been given to inculcate interdisciplinary skills that would allow the students both vertical and horizontal mobility in their progression. The faculties from the different branches of chemistry – Inorganic, Organic and Physical Chemistry had separate and joint sessions and arrived at a Draft Syllabus in Chemistry for four-semesters 2-year M.Sc. course. The Draft Syllabus was approved by the Board of Post Graduate Studies (BPGS), which constitutes of faculty members, professors from other state and central universities and cognate subject expert in a meeting held on March 31, 2015 and finally placed before the Academic Council for approval.

March 2015
Rono Hills, Itanagar

Dr. Md. Harunar Rashid
Chairman
Board of Post Graduate Studies (BPGS)
Department of Chemistry, RGU

DEPARTMENTAL PROFILE

The **Department of Chemistry** is one of the recent departments to be established by Rajiv Gandhi University in the year 2011 under the stewardship of Prof. Kamalesh Choudhury. It marked a humble beginning to impart quality teaching and research in chemistry in this remote 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 two-year (4 semesters) M.Sc. programme with specialization in all major areas of chemistry, viz. inorganic, organic and physical chemistry to provide students with the necessary theoretical background and introduction to laboratory methods. The scheme of instruction consists of lectures, tutorials, laboratory work, seminars and project work.

In addition to teaching, the department offers Ph.D. programme in chemistry. Although the department is still in its infancy, it has been striving to mark its footprint on the field of modern chemical research via its well-trained young faculties. The department is actively involved in research in frontier areas of chemistry via sponsored research projects.

March 2015
Rono Hills, Itanagar

Dr. Md. Harunar Rashid
Head (i/c)
Department of Chemistry, RGU

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:

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

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 ΣCG
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,

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

COURSE STRUCTURE

- 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).

A. 2-Year (4 Semester) M.Sc. Chemistry Course Structure

Semester	Course Code	Course Title	Maximum Marks			Credit Distribution	Credit	Total Credit
			Internal	Final Exam	Total	L : T : P		
Semester I	CHEC 401	Inorganic Chemistry I	20	80	100	3 : 1 : 0	4	**21**
	CHEC 402	Organic Chemistry I	20	80	100	3 : 1 : 0	4	
	CHEC 403	Physical Chemistry I	20	80	100	3 : 1 : 0	4	
	CHEC 404	Group Theory and Quantum Chemistry	20	80	100	3 : 1 : 0	4	
	CHEC 405	Inorganic Chemistry Laboratory	20	80	100	0 : 0 : 5	5	
Semester II	CHEC 406	Inorganic Chemistry II	20	80	100	3 : 1 : 0	4	**21**
	CHEC 407	Organic Chemistry II	20	80	100	3 : 1 : 0	4	
	CHEC 408	Physical Chemistry II	20	80	100	3 : 1 : 0	4	
	CHEC 409	Molecular Spectroscopy I	20	80	100	3 : 1 : 0	4	
	CHEC 410	Organic Chemistry Laboratory	20	80	100	0 : 0 : 5	5	
Semester III	CHEC 501	Solid State Chemistry	20	80	100	3 : 1 : 0	4	**21**
	CHEC 502	Molecular Spectroscopy II	20	80	100	3 : 1 : 0	4	
	CHEC 503	Physical Chemistry Laboratory	20	80	100	0 : 0 : 5	5	
	CHEE 5X1	Elective Course I	20	80	100	3 : 1 : 0	4	
	XXXO ###	Open Elective Course					4	
Semester IV	CHEC 504	Analytical Techniques and Computational Chemistry	20	80	100	3 : 1 : 1	5	**27**
	CHEC 505	Biochemistry	20	80	100	3 : 1 : 0	4	
	CHEE 5X2	Elective Course II	20	80	100	3 : 1 : 0	4	
	CHEE 5X3	Elective Course III	20	80	100	3 : 1 : 0	4	
	CHEE 5X4	Elective Course IV: Advanced Chemistry Laboratory & Literature Survey/Project	20	80	100	0 : 0 : 10	10	
Total Credit								**90**

B. List of Departmental Elective Courses

Specialization	Course Code	Course Title	Maximum Marks			Credit Distribution	Credit
			Internal	Final Exam	Total	L : T : P	
Inorganic	CHEE 511	Elective Course-I: Organometallic Chemistry	20	80	100	3 : 1 : 0	4
	CHEE 512	Elective Course II: Inorganic Reaction Mechanisms	20	80	100	3 : 1 : 0	4
	CHEE 513	Elective Course III: Bioinorganic Chemistry	20	80	100	3 : 1 : 0	4
	CHEE 514	Elective Course IV: Advanced Inorganic Chemistry Laboratory & Literature Survey/Project	20	80	100	0 : 0 : 10	10
Organic	CHEE 521	Elective Course I: Organic Synthesis I	20	80	100	3 : 1 : 0	4
	CHEE 522	Elective Course II: Organic Synthesis II	20	80	100	3 : 1 : 0	4
	CHEE 523	Elective Course III: Natural Products and Medicinal Chemistry	20	80	100	3 : 1 : 0	4
	CHEE 524	Elective Course IV: Advanced Organic Chemistry Laboratory & Literature Survey/Project	20	80	100	0 : 0 : 10	10
Physical	CHEE 531	Elective Course I: Physical Chemistry III	20	80	100	3 : 1 : 0	4
	CHEE 532	Elective Course II: Polymer Chemistry	20	80	100	3 : 1 : 0	4
	CHEE 533	Elective Course III: Advanced Chemical Kinetics and Photochemistry	20	80	100	3 : 1 : 0	4
	CHEE 534	Elective Course IV: Advanced Physical Chemistry Laboratory & Literature Survey/Project	20	80	100	0 : 0 : 10	10

C. List of Open Elective Courses

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

SEMESTER I

CHEC 401 Inorganic Chemistry I

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Chemical Bonding
Valance bond theory: VB treatments on homonuclear diatomic molecules (H_2 molecule); Concept of resonance, Hybrid orbital and hybridization in polyatomic molecules. Molecular Orbital Theory: LCAO-MO approach to H_2^+ ion; Molecular orbital theory of homo and hetronuclear diatomic molecules, Orbital mixing, molecular orbitals of polyatomic molecules (HF, BeH_2, H_2O, BH_3, NH_3, CH_4). Hydrogen bonding; Bonding in alloys, intermetallic compounds. Shapes of polyatomic molecules; VSEPR theory, Walsh diagram. Types of chemical bond (weak and strong), intermolecular forces.

UNIT II: Acid Base Chemistry
Lewis acid-base concept and frontier orbitals, inductive and steric effect on acidity and basicity, frustrated Lewis pair; acidity and basicity of hydrides, oxides, oxyacids of non transition elements, hard and soft acids and bases, theoretical basis of softness and hardness, HSAB principle. Applications of acid base chemistry in qualitative analysis and catalysis, superacids and superbases.

UNIT III: Main Group Chemistry
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.

UNIT IV: 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.

Recommended Books

1. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2008).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 5th Ed., Oxford University Press, New Delhi (2010).
3. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education, New Delhi (2011).

4. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 2nd Ed., Pearson Education, UK (2005).
5. Lippard, S. J.; Berg, J. M., *Principles of Bioinorganic Chemistry*, Panima Publishing Corporation, New Delhi (2005).

Further Reading

1. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2009).
2. Greenwood, N. N.; Earnshaw, A., *Chemistry of the Elements*, 2nd Ed., Reed Educational and Professional Publishing, New Delhi (2010).
3. Beritini, I.; Gray, H. B.; Lippard, S. J.; Valentine, J. S., *Bioinorganic Chemistry*, University Science Books, Mill Valley, CA (1994).
4. Roat-Malone, R. M., *Bioinorganic Chemistry: A Short Course*, 2nd Ed., John Wiley & Sons, New Jersey (2007).
5. Reddy, K. H., *Bioinorganic Chemistry*, New Age International Publishing, New Delhi (2009).

SEMESTER I

CHEC 402 Organic Chemistry I

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Conceptual Organic Chemistry
Review of basic concepts: inductive effect, electromeric effect, resonance effect, hyperconjugation, resonance. Aromaticity, non-aromaticity, homoaromaticity; Hückel's rule, n-annulenes. Applications of acid-base concept.
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 modification).

UNIT II: Stereochemistry I
Introduction to molecular symmetry and chirality, centre of chirality: molecules with C, N, S based chiral centres, asymmetry and dissymmetry, projection formulae and their interconversions. Conformational analysis of simple cyclic and acyclic systems. Molecules with more than one centre of chiral centre, concept of diastereoisomerism, diastereomerism in acyclic and cyclic system, optical purity. Chirality in molecules devoid of chiral centre-axial, planar and helical chirality.

UNIT III: Stereochemistry II
Concept of stereogenic centre, chirotopic and achirotopic centre, prochirality and prosterioisomerism, relative and absolute configuration: EZ and RS nomenclature, homotopic and heterotopic ligands and faces. Chiral synthesis, effect of conformation on reactivity (stereochemical aspects of nucleophilic addition to carbonyl compounds through various models: Cram and Felkin-anh model), chemical consequence of conformational equilibrium: Curtin Hammett priniciple.

UNIT IV: Study of Reaction Intermediates I
Carbocation: Structure and stability of carbocations, classical and non-classical carbocations, neighbouring group participation and rearrangements including Wagner-Meerwein, Pinacol-pinacolone, semi-pinacol rearrangement.
Carbanions: Generation, structure and stability. Organolithium, organomagnesium, organozinc, organocopper reagents. Mechanism of reactions involving enolate as intermediate: Michael addition, Robinson annulation, Aldol, Knoevenagel, Claisen, Stobbe condensation. Use of enol equivalent.
Free radicals: Generation, structure, stability and reactions, radical initiator. Name reactions involving radical intermediates such as Barton deoxygenation and decarboxylation, Barton reaction.

Recommended Books
1. Smith, M. B.; March, J., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 6th Ed., Wiley India, New Delhi (2012).

2. Greeves, N.; Clayden, J.; Warren, S., *Organic Chemistry*, 2nd Ed., Oxford University Press, New Delhi (2012).
3. Sengupta, S., *Basic Stereochemistry of Organic Molecules*, 1st Ed., Oxford University Press, New Delhi (2014).
4. Kalsi, P. S., *Stereochemistry: Conformation and Mechanism*, 8th Ed., New Age International Publishers, New Delhi (2015).
5. Bansal, R. K., *Synthetic Approach in Organic Chemistry*, Narosa Publishing House, New Delhi (2001).

Further Reading

1. Solomons, T. W. G.; Fryhle, C. B., *Organic Chemistry*, 10th Ed., Wiley India, New Delhi (2012).
2. Bruice, P. Y., *Organic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2009).
3. Wilen, S. H.; Eliel, E. L., *Stereochemistry of Organic Compounds*, Wiley India (2008).
4. Smith, M. B., *Organic Synthesis*, 3rd Ed., Wave Function, Inc., Irvine (2011).

SEMESTER I

CHEC 403 Physical Chemistry I

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Chemical Thermodynamics
Thermodynamics of real gases and gas mixtures: chemical potential and its variation with temperature and pressure; Gibbs-Duhem equation; Gibbs free energy and entropy of mixing of ideal gases.
Fugacity and standard state of real gases, relation between fugacity and pressure, fugacity of van der Waals gases, determination of fugacity by graphical method; variation of fugacity with temperature and pressure.
System of variable composition: partial molar quantities and its physical significance; partial molar volumes; method of determination of partial molar volumes.

UNIT II: Non–Equilibrium Thermodynamics
Postulates of non-equilibrium thermodynamics; microscopic reversibility and Onsagar's reciprocity relations; phenomenological laws and Onsagar's reciprocal relations.
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; Peltier, Seebeck and Thompson effect.

UNIT III: Chemical Kinetics I
Kinetics of complex reactions: consecutive, side and opposing reactions (first order only); steady state approximation and kinetics of simple reactions (e.g. decomposition of ozone, reaction between NO and O_2, iodination of acetone, decomposition of gaseous N_2O_5), 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.

UNIT IV: Surface Chemistry
Surface tension and surface free energy: Young-Laplace equation; pressure across curved surfaces and vapour pressure of droplets (Laplace equation, Kelvin equation).
Adsorption of gases on solid surface: Thermodynamics of adsorption; adsorption isotherms: Langmuir isotherm and BET isotherm; determination of surface area of an adsorbent (Langmuir and BET equation); isosteric enthalpy of adsorption.
Heterogeneous catalysis: Langmuir-Hinshelwood and Eley-Rideal model; kinetics of heterogeneous catalysis: unimolecular and bimolecular surface reactions.
Capillary action: Capillary condensation, adsorption in micropores and hysteresis loop. Adsorption on liquid surface: Gibb's adsorption equation and surface pressure.

Recommended Books

1. Atkins, P. W.; Paula, J. de, *Physical Chemistry,* 8th Ed., Oxford University Press, New Delhi (2006).
2. Silbey, R. J.; Alberty, R. A.; Bawendi, M. G., *Physical Chemistry*, 4th Ed., Wiley India, New Delhi (2005).
3. Levine, I. N., *Physical Chemistry*, 6th Ed. McGraw Hill Education (India), 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*, 4th Ed. Vol. 2, Macmillan Publishers India, New Delhi (2011).
7. Kapoor, K. L., *A Textbook of Physical Chemistry*, 4th Ed. Vol. 5, Macmillan Publishers India, New Delhi (2011).

Further Reading

1. Prigogine, I., *Introduction to Thermodynamics of Irreversible Processes*, 3rd Ed., Wiley (1967).
2. Adamson, A. W.; Gast, A. P., *Physical Chemistry of Surfaces,* 6th Ed, Wiley India, New Delhi (2011).
3. Shaw, D. J., *Introduction to Colloid and Surface Chemistry*, 4th Ed, Butterworths-Heinemann (1992).
4. Moudgil, H. K., *Textbook of Physical Chemistry*, PHI Learning, New Delhi (2010).

SEMESTER I

CHEC 404 Group Theory and Quantum Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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 and Mulliken notations. Direct product representation, projection operator and symmetry adapted linear combination (SALC), symmetry selection rules for IR, Raman and electronic spectra. Use of group theory in construction of hybrid orbitals (in BF_3, CH_4, $PtCl_4^{2-}$).

UNIT II: Origin of Quantum Mechanics
Failure of classical mechanics, Planck's quantum theory, Compton effect, photoelectric effect, wave particle duality, uncertainty principle.
Time-independent Schrödinger equation, properties of wave functions
Postulates of quantum mechanics; quantum mechanical operators; properties of operators; eigen values and eigen functions; setting up of operators for different observables; orbital angular momentum operators; Hermitian operators; Schmidt-orthogonalization technique.

UNIT III: Wave mechanics of some simple systems
Particle in a one dimensional box, normalization and orthogonality; characteristics of wave functions; three dimensional box; degree of degeneracy; concept of tunnelling.
Rigid rotators; simple harmonic oscillator; recursion relations of Hermite polynomials; normalization of wave functions.
Hydrogen like atom: complete solution, radial distribution function, electron spin and spin-orbit coupling.

UNIT IV: Application of Quantum Mechanics
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.
Hückel electron theory and extended Hückel MO theory and their application to ethylene, butadiene, allyl system and benzene.

Recommended Books

1. Cotton, F. A., *Chemical Applications of Group Theory*, 3rd Ed., Wiley India, New Delhi (2003).
2. Reddy, K. V., *Symmetry and Spectroscopy of Molecules*, 2nd Ed., New Age International Publishers, New Delhi (2009).

3. Chandra, A. K., *Introductory Quantum Chemistry*, 4th Ed., McGraw Hill Education (India), New Delhi (2009).
4. Levine, I. N., *Quantum Chemistry*, 6th Ed., PHI Learning, New Delhi (2012).
5. McQuarrie, D. A., *Quantum Chemistry*, Viva Books, New Delhi (2003).

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*, 4th Ed., Oxford University Press, New Delhi (2005).
3. Prasad, R. K., *Quantum Chemistry*, 4th Ed., New Age International Publishers, New Delhi (2010).

SEMESTER I

CHEC 405 Inorganic Chemistry Laboratory

5 Credit 100 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

1. Preparation and characterization by chemical analysis, IR and electronic spectrophotometry, magnetic susceptibility measurement, conductivity measurement, wherever appropriate and possible:
   (a) Potassium tris(oxalato)manganate(III) hydrate, $K_3[Mn(C_2O_4)_3]\cdot xH_2O$
   (b) Tris(acetylacetonato)iron(III), $Fe(acac)_3$
   (c) Bis(acetylacetonato)copper, $Cu(acac)_2$,
   (d) Bis(acetylacetonate)oxovanadium, $VO(acac)_2$
   (e) Bis(dimethyglyoximato)nickel(II), $Ni(dmg)_2$
   (f) Mercury tetrathiocyanato cobalt(II), $Hg[Co(NCS)_4]$
   (g) Hexammine cobalt(III) chloride, $[Co(NH_3)_6]Cl_3$
   (h) Chloropentaammine cobalt(III) chloride, $[Co(NH_3)_5Cl]Cl_2$

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. Vogel, A. I.; Mendham, J.; Denney, R. C., *Vogel's Quantitative Chemical Analysis*, 6th Ed., Pearson Education, New Delhi (2009).
2. Raj, G., *Advanced Practical Inorganic Chemistry*, Goel Publishing House, New Delhi (2011).

SEMESTER II

CHEC 406 Inorganic Chemistry II

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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

UNIT II: Magnetic properties of Transition Metal Complexes
Magnetic susceptibility, spin-only formula, spin and orbital contributions to the magnetic moment, quenching of orbital angular momentum. Effect of Temperature on magnetic moment: Curie, Curie-Weiss laws; measurement of magnetic susceptibility using Gouy and Faraday methods; Temperature Independent Paramagnetism (TIP),
Spin state cross over; magnetic properties of lanthanides and actinides. Brief review of different types of cooperative magnetic behavior.

UNIT III: Electronic Spectra of Transition Metal Complexes
Electronic Spectra of complexes: Term symbols of d^n system, Racah parameters, splitting of terms in weak and strong octahedral and tetrahedral fields. Correlation diagrams for d^n and d^{10-n} ions in octahedral and tetrahedral fields (qualitative approach), *d-d* transition, selection rules for electronic transition-effect of spin orbit coupling and vibronic coupling.
Interpretation of electronic spectra of complexes: Orgel diagrams, demerits of Orgel diagrams, Tanabe-Sugano diagrams, calculation of Dq, B and β (Nephelauxetic ratio) values, charge transfer spectra.

UNIT IV: Organometallic Chemistry
Valence electron count (18 electron rule); structure and bonding in mono and polynuclear metal carbonyls; substituted metal carbonyls and related compounds; synthesis and reactivity of metal carbonyls; vibrational spectra of metal carbonyls, metal carbonyl hydrides.
Organometallic compounds with linear π-donor ligands: synthesis, structure and bonding of olefins, acetylenes, dienes and allyl complexes.
Complexes with cyclic π-donors: Structure and bonding of metallocenes and cyclic arene complexes.

Recommended Books

1. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2008).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 5th Ed., Oxford University Press, New Delhi (2010).

3. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education, New Delhi (2011).
4. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 2nd Ed., Pearson Education, UK (2005).
5. Mehrotra, R. C.; Singh, A., *Organometallic Chemistry: A Unified Approach*, New Age International Publishers, New Delhi (2014).
6. Crabtree, R. H., *The Organometallic Chemistry of the Transition Metals*, John Wiley & Sons, New Jersey (2005).

Further Reading

1. Figgis, B. N.; Hitchman, M. A., *Introduction to Ligand Field Theory and Its Applications*, Wiley India, New Delhi (2010).
2. Elschenbroich, C., *Organometallics*, 3rd Ed., Wiley-VCH, Weinheim (2006).
3. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2007).
4. Sathyanarayana, D. N., *Electronic Absorption Spectroscopy and Related Techniques*, Universities Press, Hyderabad (2001).

SEMESTER II

CHEC 407 Organic Chemistry II

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Study of Reaction Intermediates II
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: Curtius, Hoffmann, Schmidt, Lossen, Beckmann rearrangement reactions.
Ylides: Chemistry of phosphorous and sulfur ylides - Wittig and related reactions.
Arynes: Generation, structure and stability, rearrangement reactions, trapping of benzynes.
Enamine: Generation and reactions of enamines, Stork enamine reaction.

UNIT II: 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.
Addition Reactions: Mechanism and stereochemical aspects of addition reactions in carbon-carbon multiple bonds.

UNIT III: Oxidation and Reduction
Oxidation: Metal and non-metal based oxidations of a) alcohols to carbonyls (Chromium, manganese, aluminium, silver, DMSO, hypervalent iodine and TEMPO based reagents); b) oxidation of phenols: Fremy's salt c) alkenes to epoxides: via halohydrin, peroxides/per acids based, Sharpless asymmetric epoxidation; d) alkenes to diols (Manganese, osmium based), Prevost reaction and Woodward modification; d) alkenes to carbonyls: ozonolysis, use of mercuric acetate; e) cleavage of 1,2-diols: lead tetraacetate, sodium periodate; f) oxidation of alkyl or alkenyl fragments: selenium dioxide; g) ketones to ester/lactones: Baeyer-Villiger oxidation.
Reduction: a) Catalytic hydrogenation (Heterogeneous: Palladium/ Platinum/ Rhodium/ Nickel etc; Homogeneous: Wilkinson); b) metal-liquid ammonia processes: Birch reduction, Pinacol formation etc.; c) stereo selection and mechanism of the following reagents: Lithium aluminium hydride, L-selectride, K-selectride, Sodium borohydride, DIBAL, sodium cyanoborohydride, Alkyl borane, tributyltin hydride; d) non-metallic reducing agents: diimide, hydrazine (Wolff-Kishner reduction); e) reduction with aluminium compounds: Meerwin-Ponndorf-Verley reduction.

UNIT IV: Pericyclic Reactions
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 Books

1. Bansal, R. K., *Synthetic Approach in Organic Chemistry*, Narosa Publishing House, New Delhi (2001).
2. Smith, M. B.; March, J., *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 6th Ed., Wiley India, New Delhi (2012).
3. Smith, M. B., *Organic Synthesis*, 3rd Ed., Wave Function, Inc., Irvine, (2010).
4. Greeves, N.; Clayden, J.; Warren, S., *Organic Chemistry*, 2nd Ed., Oxford University Press, New Delhi (2012).
5. Sengupta, S., *Basic Stereochemistry of Organic Molecules*, 1st Ed., Oxford University Press, New Delhi (2014).

Further Reading

1. Carruthers, W., *Modern Methods of Organic Synthesis*, 4th Ed., Cambridge University Press, New Delhi (2005).
2. Solomons, T. W. G.; Fryhle, C. B., *Organic Chemistry*, 10th Ed., Wiley India, New Delhi (2012).
3. Bruice, P. Y., *Organic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2009).
4. Mukherjee, S. M.; Singh, S. P., *Reaction Mechanism in Organic Chemistry*, Macmillan Publishers India, New Delhi (2010).
5. Singh, J.; Singh, J. *Photochemistry and Pericyclic Reactions*, New Age International Publishers, New Delhi (2010).

SEMESTER II

CHEC 408 Physical Chemistry II

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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
Activity and activity coefficient of ions in solution; 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
Polymers: Classification and types of polymers. Concept and types of molecular weight; derivation of number and mass average molecular weight; polydispersity and distribution of molecular weight in polymers; significance of molecular weight; degree of polymerization and chain length.
Methods of determining molecular weights of macromolecules: osmometry, viscometry and light scattering methods.
Types of polymerization; kinetics of addition and step growth (condensation) polymerisation.

Distribution of chain lengths: random walk model and average end-to-end, root mean square end-to-end and most probable end-to-end chain length; freely jointed chain model.

Recommended Books

1. Gupta, M. C., *Statistical thermodynamics,* New Age International Publishers, New Delhi (2007).
2. Levine, I. N., *Physical Chemistry*, 6th Ed. McGraw Hill Education (India), New Delhi (2011).
3. Kapoor, K. L., *A Textbook of Physical Chemistry*, 4th Ed. Vol. 5, Macmillan Publishers India, New Delhi (2011).
4. Laidler, K. J., *Chemical Kinetics*, 3rd Ed., Pearson Education, New Delhi (2011).
5. Bockris, J. O. M.; Reddy, A. K. N., *Modern Electrochemistry*, 2nd Ed., Vol. 1, Springer India, New Delhi (2006).
6. Bockris, J. O. M.; Reddy, A. K. N., *Modern Electrochemistry*, 2nd Ed., Vol. 2, Springer India, New Delhi (2006).

Further Reading

1. McQuarrie, D. A., *Statistical Mechanics*, Viva Books, New Delhi (2003).
2. Atkins, P. W.; Paula, J. de, *Physical Chemistry,* 8th Ed., Oxford University Press, New Delhi (2006).
3. Glasstone, S., *An Introduction to Electrochemistry*, Nabu Press, India (2011).
4. Gowariker, V. R., Viswanathan, N. V. and Sreedhar, J., *Polymer Science*, New Age International Publishers, New Delhi (2011).
5. Billmeyer, F. W., *Textbook of Polymer Science*, Wiley India, New Delhi (2010).
6. Moudgil, H. K., *Textbook of Physical Chemistry*, PHI Learning, New Delhi (2010).

SEMESTER II

CHEC 409 Molecular Spectroscopy I

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Basics of Molecular Spectroscopy
Electromagnetic spectrum, interaction of electromagnetic radiation with molecular systems. Spectroscopic transition-absorption, emission, reflection, polarisation and scattering processes, transition probability, transition dipole moments and selection rules. Width and intensity of spectral transitions, Signal-to-noise ratio, fourier transformation in spectroscopy, Laser and Laser spectroscopy.

UNIT II: Rotational (Microwave) Spectroscopy
Rotational spectra of diatomic and polyatomic molecules. Intensities of rotational spectral lines, effect of isotopic substitution. Non-rigid rotators.
Pure rotational Raman spectra. Rotational-rotational and rotational-vibrational transitions. Polarisation of Raman lines, specific selection rules in Raman spectroscopy, Stokes and anti-Stokes lines.

UNIT III: Vibrational Spectroscopy
Simple harmonic oscillators - wave functions and energies, anharmonic oscillators. Interaction of rotation and vibrations, diatomic vibrating rotators (carbon monoxide), Vibrations of polyatomic molecules – symmetry properties, overtone and combination frequencies. Influence of rotation on vibrational spectra.
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.
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.

UNIT IV: Electronic spectroscopy
Electronic spectroscopy of diatomic molecules, Frank-Condon principle, dissociation and predissociation spectra. Rotational fine structure. Spectrum of molecular hydrogen. Change of shape on excitation. $\pi-\pi$, $n-\pi$, and *d-d* transitions and their selection rules.
UV-Vis spectroscopy: λ_{max} and molar absorptivity, factors affecting them. Calculation of λ_{max},Woodward-Fieser rule.

Recommended Books

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 4th Ed., Cengage Learning India, New Delhi (2012).
2. Banwell C. N.; McCash, E. M., *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill, New Delhi (2011).
3. Drago, R. S., *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing, Florida (1999).

4. Dyer, J. R., *Applications of Spectroscopy of Organic Compounds*, PHI Learning, New Delhi (2004).
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., John Wiley & Sons, New Jersey (2009).
2. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds*, *Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry*, 6th Ed., John Wiley & Sons, New Jersey (2009).
3. Gunther, H., *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Ed., Wiley India, New Delhi (1995).
4. Silverstein, R. M.; Webster, F. X., *Spectrometric Identification of Organic Compounds*, 6th Ed., Wiley India, New Delhi (2005).
5. William D. H.; Fleming, I., *Spectroscopic Methods in Organic Chemistry*, 6th Ed., McGraw Hill Education (India), New Delhi (2011).
6. Aruldas, G., *Molecular Structure and Spectroscopy*, 2nd Ed., PHI Learning, New Delhi (2007).

SEMESTER II

CHEC 410 Organic Chemistry Laboratory

5 Credit 100 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

1. Qualitative Organic Analysis (Maximum three samples) of supplied organic binary mixtures:
   (a) qualitative separation by physico-chemical method,
   (b) identification of the compounds by chemical analysis,
   (c) preparation of suitable derivatives, purification and determine melting point.

2. Chromatographic (TLC & Paper) identification of organic compounds. (Nitro compounds, amino acids and any other binary mixture)

3. Isolation of natural products
   (a) Caffeine from tea leaves
   (b) Nicotine from tobacco
   (c) β-Carotene from carrot/ tomato
   (d) Casein from milk
   (e) Any other extraction possible in the laboratory

Recommended Books

1. Mann, F. G., *Practical Organic Chemistry*, 4th Ed., Pearson Education India, New Delhi (2009).
2. Clarke, H. T., *A Handbook of Organic Analysis: Qualitative and Quantitative*, CBS Publishers, New Delhi (2007).
3. Agarwal, O. P., *Advanced Practical Organic Chemistry*, Goel Publishing House, New Delhi (2010).
4. 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 (2005).

SEMESTER III

CHEC 501 Solid State Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: 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, packing efficiency, 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: ABO_3, K_2NiF_4 and spinels. Lattice enthalpy, consequences of lattice enthalpy.
Crystal defects: Types of defect: point defects, line defect and plane defect, thermodynamics of Schottky and Frenkel defect formation.

UNIT II: Preparation and Characterization of solids
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).
X-ray diffraction methods: Powder diffraction, uses of powder diffraction, structure determination from XRD, crystallite size, Rietveld method; Single crystal X-ray analysis, structure factor, phase problem.
Electron microscopy: Principles and application of scanning electron microscopy (SEM), transmission electron microscopy (TEM), energy dispersive analysis of X-rays (EDAX).

UNIT III: Properties of Solids
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; select magnetic materials such as metal monoxides, spinels, ferrites and perovskites; 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; Superconducting compounds-structural aspects; Superconductivity in cuprates, preparation and characterization of 1-2-3 materials. Applications of high Tc materials. Organic superconductors, Fullerenes and doped fullerenes as superconductors.
Intercalation compounds of graphite, zirconium and transition metal chalcogenide; Polymer-clay nanocomposites, Carbon-Carbon and polymer composite.

Recommended Books

1. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2008).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 5th Ed., Oxford University Press, New Delhi (2010).
3. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education, New Delhi (2011).
4. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 2nd Ed., Pearson Education, UK (2005).
5. Smart, L. E.; Moore, E. A., *Solid State Chemistry: An Introduction*, 3rd Ed., CRC Press, New Delhi (2010).
6. West, A. R., *Solid State Chemistry and its Application*, Wiley India, New Delhi (2011).
7. Kakani, S. L.; Kakani, A., *Materials Science*, 2nd Ed., New Age International Publishers, New Delhi (2010).

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*, New Age International Publishers, New Delhi (2011).

SEMESTER III

CHEC 502 Molecular Spectroscopy II

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I : NMR Spectroscopy
Basic principles, origin of chemical shift, spin-spin coupling, relaxation processes, first order spectra. Spin decoupling and NOE. Applications of ^{1}H and ^{13}C in simple organic molecules. Brief introduction to 2D NMR – COSY, NOESY.
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.

UNIT II: Mössbauer and NQR Spectroscopy
Mössbauer Spectroscopy: Basic principles, Doppler shift, recoil energy, isomer shift and interpretation. Quadrupole coupling. Applications to the studies of (a) bonding and structures of Fe^{2+} and Fe^{3+} compounds (b) metal carbonyls, (c) Sn^{2+} and Sn^{4+} compounds and (d) Iodine.
NQR Spectroscopy: Basic principles, electric field gradient (EFG), asymmetry parameter, effect of magnetic field. Application of NQR in transition metal complexes.

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: 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, contact and dipolar mechanism. 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.

Recommended Books

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 4th Ed., Cengage Learning India, New Delhi (2012).
2. Banwell C. N.; McCash, E. M., *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill, New Delhi (2011).

3. Drago, R. S., *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing (1999).
4. Dyer, J. R., *Applications of Spectroscopy of Organic Compounds*, PHI Learning, New Delhi (2004).
5. Kemp, W., *Organic Spectroscopy*, 3rd Ed., Macmillan Publishers India, New Delhi (2011).

Further Reading

1. Gunther, H., *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Ed., Wiley India, New Delhi (1995).
2. Silverstein, R. M.; Webster, F. X., *Spectrometric Identification of Organic Compounds*, 6th Ed., Wiley India, New Delhi (2005).
3. William D. H.; Fleming, I., *Spectroscopic Methods in Organic Chemistry*, 6th Ed., McGraw Hill Education (India), New Delhi (2011).
4. Aruldas, G., *Molecular Structure and Spectroscopy*, 2nd Ed., PHI Learning, New Delhi (2007).

SEMESTER III

CHEC 503 Physical Chemistry Laboratory

5 Credit 100 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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 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's 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.

Recommended Books

1. James, A. M.; Prichard, F. E., *Practical Physical Chemistry*, 3rd Ed., Prentice Hall Press (1974).
2. Viswanathan, B.; Raghavan, P. S., *Practical Physical Chemistry*, Viva Books, New Delhi (2012).
3. Yadav, J. B., *Advanced Practical Physical Chemistry*, 33rd Ed., Goel Publishing House (2013).
4. Das, R. C.; Behera, B., *Experimental Physical Chemistry*, McGraw Hill Education (India), New Delhi (1984).

SEMESTER III

CHEE 511 ELECTIVE I: Organometallic Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Organometallic Compounds containing M=C and M≡C Bonds
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 carbene complexes: synthesis, structure and reactivity

UNIT II: 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 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: Metal-Metal Bond and Clusters
Definition of metal clusters, metal-metal multiple bonding in $[M_2X_8]^{2-}$, high nuclearity metal halide clusters.
Low nuclearity metal-carbonyl clusters, high nuclearity metal-carbonyl clusters with internal atoms. Structure, synthesis and reactivity. Wade's rule (PSEPT), capping rules, isolobal relationships between main-group and transition metal fragments.
Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters. Molecular clusters in catalysis.

Recommended Books

1. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2008).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 5th Ed., Oxford University Press, New Delhi (2010).

3. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education, New Delhi (2011).
4. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 2nd Ed., Pearson Education, UK (2005).
5. Mehrotra, R. C.; Singh, A., *Organometallic Chemistry: A Unified Approach*, New Age International Publishers, New Delhi (2014).
6. Crabtree, R. H., *The Organometallic Chemistry of the Transition Metals*, John Wiley & Sons, New Jersey (2005).

Further Reading

1. Elschenbroich, C., *Organometallics*, 3rd Ed., Wiley-VCH, Weinheim (2006).
2. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2007).
3. Jordan, R. B.; *Reaction Mechanisms of Inorganic and Organometallic Systems*, 3rd Ed., Oxford University Press, New York (2007)

SEMESTER III

CHEE 521 ELECTIVE I: Organic Synthesis I

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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 group and two group C-X disconnections, chemoselectivity, reversal of polarity, cyclisation reactions, amine synthesis. One group C-C disconnections – alcohols and carbonyl compounds, regioselectiviity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis. 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: Protection and Deprotection Chemistry
Protection and deprotection of hydroxy, carboxyl, carbonyl, carboxy amino groups and carbon-carbon multiple bonds; chemo- and regioselective protection and deprotection; illustration of protection and deprotection in synthesis.

UNIT III: Heterocyclic Chemistry
a) Small Ring Heterocycles: Syntheses of aziranes, oxiranes & thiiranes; ring openings and heteroatom extrusion; synthesis & reactions of azetidines, oxetanes & thietanes.
b) Aromatic heterocycles: Synthesis and reactions of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole. Concept of π-excessive and π-deficient heterocyclics.
c) Condensed Five-membered Rings (1 Heteroatom): Synthesis and reactions of indole, benzofuran and benzothiophene.
d) Diazines: Structural & chemical properties; Synthesis of pyridazines, pyrimidines, pyrazines, nucleophilic and electrophilic substitutions.

UNIT IV: Photoorganic Chemistry
Photochemistry: Introduction, excited states, cis-trans isomerisation, Norrish type I & II reaction, photoreduction of ketones, Paterno-Buchi reaction, Di- π-methane and Di-π-methane type rearrangement, photo Fries rearrangement, Barton reaction, Hoffmann-Loeffler-Freytag raction.

Recommended Books

1. Warren, S., *Organic Synthesis: The Disconnection Approach*, Wiley India, New Delhi (2010).
2. Ghosh, S. K. *Advanced General Organic Chemistry: A Modern Approach, Part-II*, New Central Book Agency, Kolkata (2009).
3. Greeves, N.; Clayden, J.; Warren, S., *Organic Chemistry*, 2nd Ed., Oxford University Press, New Delhi (2012).

4. Mukherjee, S. M.; Singh, S. P.; Kapoor, R. P., *Organic Chemistry*, Vol. III, New Age International Publishers, New Delhi, (2009).
5. Singh, J.; Singh, J. *Photochemistry and Pericyclic Reactions*, New Age International Publishers, New Delhi (2010).
6. Smith, M. B., *Organic Synthesis*, 3rd Ed., Wave Function, Inc., Irvine, (2011).

Further Reading

1. Willis, C.; Willis, M., *Organic Synthesis*, Oxford Chemistry Primers, Oxford University Press, UK (1995).
2. Kocieński, P. J., *Protecting Groups*, 3rd Ed., Thieme Georg Verlag, (2005).
3. Gilchirst, T. L., *Heterocyclic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2005).
4. DePuy, C. H.; Chapman, O. L., *Molecular Reactions and Photochemistry*, PHI Learning, New Delhi (1988).

SEMESTER III

CHEE 531 ELECTIVE I: Physical Chemistry III

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Application of Quantum Mechanics
Electron spin and hydrogen atom; Pauli principle and helium atom; Slater determinant.
Hartree-Fock self-consistent-field method; Hartree–Fock treatment of atoms.
Valence bond (VB) and molecular orbital (MO) treatment of diatomic molecules; Born-Oppenheimer approximation; LCAO approximation; LCAO applies to H_2^+ and H_2 molecules; VB treatment of H_2 molecules.
The Virial theorem and Hellmann–Feynmann theorem; hybridization and shapes of orbital: hybrid orbitals in terms of wave functions of s and p orbitals (sp, sp^2 and sp^3 hybridization).

Unit II: Application of Statistical Thermodynamics
Equilibrium constant of a reaction in terms of partition function; transition state theory; monoatomic solids: Einstein and Debye theory; thermodynamic properties of solids; statistical treatment of the black–body radiations; statistical mechanics of independent particles: localized and non-localized particles; van der Walals approximation and statistical thermodynamics.

UNIT III: Catalysis by Surfaces
Acidity and basicity of catalysts; thermodynamics of catalysed reactions, heat and mass transport limitations, conversion and selectivity.
The selectivity of catalyst; catalytic activity: turn over frequency and turn over number; Volcano plots; catalyst deactivation: coking and carbon deposition; catalyst poisoning and promotion; regenerative treatment of deactivated catalyst; catalytic converters.
Catalyst in energy conversion and in production of hydrocarbon feedstocks; hydrodesulphurization; production of chemicals from synthetic gas; catalytic cracking and reforming; catalysts in atmospheric pollution control.

UNIT IV: Characterization of Catalysts and Their Surfaces
Importance of pore structure and surface area; methods of estimating surface areas: volumetric method and gas adsorption method.
Surface characterization techniques such as X-ray fluorescence (XRF); X-ray diffraction (XRD); secondary ions mass spectrometry (SIMS); infra-red spectroscopy (IR); high energy electron energy loss spectroscopy (HREELS); photoelectron spectroscopy (PES); low energy electron diffraction (LEED); extended X-ray absorption fine structure (EXAFS); X-ray absorption near edge structure (XANES); temperature programmed desorption (TPD).

Recommended Books

1. Chandra, A. K., *Introductory Quantum Chemistry*, 4th Ed., McGraw Hill Education (India), New Delhi (2009).
2. Levine, I. N., *Quantum Chemistry*, 6th Ed., PHI Learning, New Delhi (2012).
3. McQuarrie, D. A., *Quantum Chemistry*, Viva Books, New Delhi (2003).
4. Bond G. C., *Heterogeneous Catalysis: Principle and Application*, 2nd Ed., Oxford University Press (1987).
5. Gates B. C., *Catalytic Chemistry*, John Wiley and Sons, New Jersey (1992).
6. Thomas, J. M.; Thomas, W. J., *Principle and Practice of Heterogeneous Catalysis*, Wiley-VCH, Weinheim (1996).

Further Reading

1. Barthalomew, C. H.; Farrauto R. J., *Fundamentals of Industrial Catalytic Processes*, John Wiley & Sons, New Jersey (2006).
2. Chakrabarty, D. K.; Viswanathan, B., *Heterogeneous Catalysis*, New Age International Publishers, New Delhi (2008).
3. Viswanathan B.; Kannan, S.; Deka, R. C., *Catalysts and Surfaces Characterization Techniques*, Narosa Publishing House, New Delhi (2010).

SEMESTER IV

CHEC 504 Analytical Techniques and Computational Chemistry

5 Credit 60 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Electrochemical and Radiochemical Methods
Electrochemical methods: Principles, instrumentation and applications of coulometry, polarography, polarographic cell, polarogamm, polarographic waves, dropping mercury electrode, cyclic voltammetry, electrogravimetry.
Radiochemical methods: Tracers in chemical analysis, isotopic exchange, isotopic dilution technique, labeling experiments in studying reaction mechanism.

UNIT II: Analytical Techniques
Solvent extraction: principle and technique, distillation coefficient.
Thermal analysis: Thermogravimetry (TG), evolved gas analysis and detection, derivative thermogravimetry (DTG), differential thermal analysis (DTA), temperature programmed desorption (TPD) and differential scanning calorimetry (DSC) - principles and applications.
Principles of X-ray photoelectron spectroscopy (XPS), Auger electron spectroscopy (AES), ESCA and their applications. Principles of atomic absorption spectroscopy and applications.

UNIT III Numerical and Computational Methods
Regression analysis, least squares method, Curve fitting (least square), solution of polynomial equation, numerical integration (Trapezoidal rule, Simpson's rule, Gaussian quadrature), solution of ordinary differential equations (Euler's method, Runge-Kutta method, predictor-corrector method), matrix multiplication, inversion and diagonalisation.
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.

UNIT IV: 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 draw a moderately complex molecule e.g., aniline/ pyridine/ furan/ ethylenediamine using PC model and obtaining its nuclear framework Z-matrix in usual MOPAC form.
3. 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.

4. To find rotational probability distribution for HCl at two different temperatures and compare its rotational partition function by direct calculation and by applying simple formula.
5. *Ab-initio* calculations of organic and inorganic molecules using GAUSSIAN software.
6. Spectral interpretation of organic compounds via UV, IR and NMR spectra of the following:
   a) 1,3,5-Trimethyl benzene
   b) Pinacolone
   c) *n*-Propylamine
   d) *p*-Methoxy benzyl alcohol
   e) Benzyl bromide
   f) Phenylacetone
   g) 2-Methoxyethyl acetate
   h) Acetone
   i) Isopropyl alcohol
   j) Pyridine
   k) 4-Picoline
   l) 1,3-Dibromo-1,1-dichloropropene
   m) Cinnamaldehyde

Recommended Books

1. Bard, A. J.; Faulkner, L. R.; *Electrochemical Methods: Fundamentals and Application*, 2nd Ed., Wiley India, New Delhi (2006).
2. Braun, R. D.; *Introduction to Instrumental Analysis*, 2nd Ed., BSP Books, Hyderabad (2011).
3. Willard, H. H.; Merritt, L. L.; Dean, J. A.; Settle, F. A., *Instrumental Methods of Analysis*, 7th Ed., CBS Publisher, New Delhi (2012).
4. Drago, R. S., *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing, Florida (1999).
5. Balagurusamy, E., *Numerical Methods*, Tata McGraw Hill, New Delhi (1999).

Further Reading

1. Rajaram, V., *Computer Programming in FORTRAN 77*, 4th Ed., PHI Learning, New Delhi (2009).
2. Rajaram, V., *Computer Oriented Numerical Methods*, 3rd Ed., PHI Learning, New Delhi (2004).

SEMESTER IV

CHEC 505 Biochemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Chemistry of Carbohydrates
Monosaccharides: Classification, D and L series, Reaction of monosaccharides-epimerization, enediol rearrangement, oxidation, reduction, glycosylation, osazone formation. Determination of ring size- reaction with periodic acid, lead tetraacetate. Methods of descending/ascending the sugar series, interconversion of aldose and ketose. Structure of glucose and fructose.
Disaccharides: Ring structure of cellobiose, maltose, lactose, gentiobiose, sucrose, and their hydrolysis.
Polysaccharides: Introduction to starch, cellulose, glycogen, dextran and sialic acid; Cell-cell recognition and blood group substances.

UNIT II: Metabolism and its Regulation
Glycolysis, fate of pyruvate under anaerobic condition, TCA cycle and gluconeogenesis. Electron transport and oxidative phosphorylation.

UNIT III: Amino Acids and Enzymes
Types of amino acids; amphoteric behavior; definition of polypeptides and enzymes. Primary, secondary and tertiary and quaternary structures of enzymes, mechanism of enzyme action. Role of co-enzymes in biological reactions.
Protein conformations– globular and fibrous. Ramachandran plot. Protein folding and denaturation.

UNIT IV: Lipids and Nucleic Acids
Definition, nature, biological importance of fatty acids and lipids, even chain and odd chain fatty acids, 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, DNA Replication, Types of RNA. Role of DNA and RNA in protein biosynthesis. Genetic code and basis of hereditary. Gene mutation and carcinogenesis.

Recommended Books

1. Wade, L. G. Jr., *Organic Chemistry*, 8th Ed., Pearson Education, Illinois (2013).
2. Cox, M. M.; Nelson, D. L., *Lehninger Principles of Biochemistry*, 6th Ed., W. H. Freeman, New York (2013).
3. Berg, J. M.; Tymoczko, J. L.; Stryer, L., *Biochemistry*, 7th Ed., W. H. Freeman, New York (2012).
4. Voet, D.; Voet, J. G., *Biochemistry*, 4th Ed., John Wiley and Sons, New Jersey (2011).

Further Reading

1. Campbell, M. K.; Farrell, S. O., *Biochemistry*, 7th Ed., Cengage Learning, Belmont (2012).
2. Metzler, D. E., *Biochemistry: The Chemical Reactions of Living Cells*, 2nd Ed., Elsevier Academic Press (2003).

SEMESTER IV

CHEE 512 ELECTIVE II: Inorganic Reaction Mechanisms

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Metal-Ligand Equilibria in Solution
Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate effect, macrocyclic effect and their thermodynamic origin. Determination of stability constant by Job's and Bjerrum methods.

UNIT II: 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 III: Electron Transfer Reactions
Classification of reactions: complementary and non-complementary reaction, 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.

UNIT IV: Photochemical Reactions
Photochemical processes, Kasha's rule, quantum yield, Jabolnskii diagrams, prompt and delayed reaction, *d-d* and charge transfer reactions, photo substitution and photo-redox reactions of cobalt, rhodium, chromium and complexes, ligand photoreactions and solar energy conversion.

Recommended Books

1. Miessler, G.; Tarr, D. A., *Inorganic Chemistry*, 3rd Ed., Pearson Education, New Delhi (2008).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 5th Ed., Oxford University Press, New Delhi (2010).
3. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education, New Delhi (2011).
4. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 2nd Ed., Pearson Education, UK (2005).

Further Reading

1. Jordan, R. B.; *Reaction Mechanisms of Inorganic and Organometallic Systems*, 3rd Ed., Oxford University Press, New York (2007).
2. Cotton, F. A.; Bochmann, M.; Murillo, C. A.; Wilkinson, G., *Advanced Inorganic Chemistry*, 6th Ed., Wiley India, New Delhi (2007).

SEMESTER IV

CHEE 513 ELECTIVE III: Bioinorganic Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: 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 II: Molybdenum and Copper-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.

UNIT III: Zinc and Cobalt-Containing Enzymes
Zinc-containing enzymes: zinc fingers, carbonic anhydrase, carboxy peptidase, 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. Lippard, S. J.; Berg, J. M., *Principles of Bioinorganic Chemistry*, Panima Publishing Corporation, New Delhi (2005).
2. Atkins, P.; Overton, T.; Rouke, J.; Weller, M.; Armstrong, F.; Hagerman, M., *Shriver Atkins's Inorganic Chemistry*, 5th Ed., Oxford University Press, New Delhi (2010).
3. Huheey, J. E.; Keiter, E. A.; Keiter, R. L.; Medhi, O. K., *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Ed., Pearson Education, New Delhi (2011).
4. Housecroft, C. E; Sharpe, A. G., *Inorganic Chemistry*, 2nd Ed., Pearson Education, UK (2005).

Further Reading

1. Beritini, I.; Gray, H. B.; Lippard, S. J.; Valentine, J. S., *Bioinorganic Chemistry*, University Science Books, Mill Valley, CA (1994).
2. Roat-Malone, R. M., *Bioinorganic Chemistry: A Short Course*, 2nd Ed., John Wiley & Sons, New Jersey (2007).
3. Berg, J. M.; Tymoczko, J. L.; Stryer, L., *Biochemistry*, 7th Ed., W. H. Freeman, New York (2012).
4. Voet, D.; Voet, J. G., *Biochemistry*, 4th Ed., John Wiley and Sons, New Jersey (2011).
5. Reddy, K. H., *Bioinorganic Chemistry*, New Age International Publishing, New Delhi (2009).

SEMESTER IV

CHEE 514 ELECTIVE IV

Advanced Inorganic Chemistry Laboratory

Total Marks: 100 (Internal 20 + End Semester Exam 80)
5 Credit 100 Contact Hours

1. Preparation and identification of the following inorganic complexes by spectroscopic (electronic and FT-IR) measurements:
   a) Synthesis of Schiff's base ligands and their complexation with transition metals.
   b) Synthesis of dithiocarbamate ligands and their complexation with transition metals.
   c) Synthesis of $M(acac)_3$ where M = Mn, Co.
   d) Synthesis of Prussian Blue.
   e) Linkage isomers of nitro and nitritopentamminecobalt(III) chloride.
   f) Optical isomers of tris(ethylenediamine)cobalt(III)chloride

2. Preparation of:
   a) Nanoparticles by sol-gel/ coprecipitation method.
   b) Metal ceramic particles.

3. 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.

Recommended Books

1. Vogel, A. I.; Mendham, J.; Denney, R. C., *Vogel's Quantitative Chemical Analysis*, 6th Ed., Pearson Education, New Delhi (2009).
2. Raj, G., *Advanced Practical Inorganic Chemistry*, Goel Publishing House, New Delhi (2011).

Literature Survey (5 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.

Project Work (10 Credit)

- Project work would be in lieu of Advanced Inorganic Chemistry Laboratory and Literature Survey.
- 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).

SEMESTER IV

CHEE 522 ELECTIVE II: Organic Synthesis II

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Asymmetric Synthesis
Introduction, asymmetric induction: substrate, reagent and catalyst controlled reactions, use of chiral auxiliaries, Sharpless asymmetric dihydroxylation, Noyori asymmetric hydrogenation, Jacobsen epoxidation, Shi epoxidation, Sharpless asymmetric aminohydroxylation.

UNIT II: Advanced Topics in Stereochemistry
a) Conformations of cyclic organic molecules: conformations of fused polycyclic systems: decalin, 1-decalone, 2-decalone, perhydroanthracene, ring size and easy of cyclisation, Baldwin's rules for cyclisation reactions.
b) 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, ceric ammonium nitrate, Gilman's reagent, lithium disopropylamide, dicyclohexylcarbodimide, trimethysilyl iodide, 1,3-dithiane reactivity: Umpolung effect, Phase transfer catalyst, Tebbe reagent, Baker's yeast, NBS, Mosher's reagent, DDQ.

UNIT IV: Modern Synthetic Methods
Biginelli reaction, Hantzsch reaction, Ugi reaction, McMurry olefination, Grubb's reaction, Mitsonobu reaction, Nef reaction, Peterson's olefination, Henry reaction, Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi, Sonogashira, Buchwald-Hartwig, Ullmann coupling reactions.

Recommended Books

1. Greeves, N.; Clayden, J.; Warren, S., *Organic Chemistry*, 2nd Ed., Oxford University Press, New Delhi (2012).
2. Sengupta, S., *Basic Stereochemistry of Organic Molecules*, 1st Ed., Oxford University Press, New Delhi (2014).
3. Carruthers, W., *Modern Methods of Organic Synthesis*, 4th Ed., Cambridge University Press, New Delhi, (2005).

Further Reading

1. Smith, M. B., *Organic Synthesis*, 3rd Ed., Wave Function, Inc., Irvine, (2010).

SEMESTER IV

CHEE 523 ELECTIVE III: Natural Products and Medicinal Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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.
ADMET of drugs: Factors affecting Absorption, Distribution, Metabolism, Elimination and Toxicity.

UNIT IV: Natural Products in Drug Discovery
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.
Sources (Plant, animal, microbial, marine) of natural products, 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 methods. Natural products as medicinal agents along with their structurally modified form: Artemisinin, Ephedrines, Ergot alkaloids, Vasicine, Taxol.

Recommended Books

1. Finar, I. L. *Organic Chemistry,* 5th Ed., Vol. 2, Pearson Education, New Delhi (2011).
2. Agarwal, O. P. *Chemistry of Organic Natural Products,* 41st Ed., Vol. I, Goel Publishing House, New Delhi (2014).
3. Agarwal, O. P. *Chemistry of Organic Natural Products, ,* 41st Ed., Vol. II, Goel Publishing House, New Delhi (2014).
4. Patrick, G. L., *An Introduction to Medicinal Chemistry*. 5rd Ed.; Oxford University Press, New Delhi (2013).

5. Silverman, R. B., *The Organic Chemistry of Drug Design and Drug Action*, 2nd Ed.; Elsevier Academic Press (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. Williams, D. A.; Lemke, T. L., *Foye's Principles of Medicinal Chemistry*. 6th Ed., Lippincott Williams and Willkins (2006).

SEMESTER IV

CHEE 524 ELECTIVE IV

Advanced Organic Chemistry Laboratory

Total Marks: 100 (Internal 20 + End Semester Exam 80)
5 Credit 100 Contact Hours

1. Separation of supplied organic binary mixtures by chromatographic means and identification of functional groups using spectroscopic tools.

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

3. Greener practice in organic synthesis:
   (a) Acetylation of primary amine
   (b) Bromination of acetanilide
   (c) Nitration of phenol
   (d) Pinacol Pinacolone rearrangement

Books Recommended

1. Chatwal, G. R., Anand, S. K. *Instrumental Methods of Chemical Analysis*, Himalaya Publishing House, India, (2010).
2. Agarwal, O. P., *Advanced Practical Organic Chemistry*, Goel Publishing House, India, (2010).
3. Monograph on Green Chemistry Laboratory Experiments, Green Chemistry Task Force Committee, DST.
4. 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).

New innovative experiments may be introduced from time to time.

Literature Survey (5 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.

Project Work (10 Credit)

- Project work would be in lieu of Advanced Organic Chemistry Laboratory and Literature Survey.

- 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).

SEMESTER IV

CHEE 532 ELECTIVE II: Polymer Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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, New Delhi (2008).
2. Billmeyer, F. W., *Textbook of Polymer Science*, Wiley India, New Delhi (2010).

SEMESTER IV

CHEE 533 ELECTIVE III: Advanced Chemical Kinetics and Photochemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Study of Chemical Reactions
Methods of studying chemicals 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 (2009).
3. Rohatgi-Mukherjee, K. K., *Fundamentals of Photochemistry*, 3rd Ed., New Age International Publishers, New Delhi (2014).

Further Reading

1. Pilling, M. J.; Pilling, S.; Seakins, P. W., *Reaction Kinetics*, Oxford University Press, USA (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 534 ELECTIVE IV

Advanced Physical Chemistry Laboratory

Total Marks: 100 (Internal 20 + End Semester Exam 80)
5 Credit 100 Contact Hours

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.

Recommended Books

1. James, A. M.; Prichard, F. E., *Practical Physical Chemistry*, 3rd Ed., Prentice Hall Press (1974).
2. Viswanathan, B.; Raghavan, P. S., *Practical Physical Chemistry*, Viva Books, New Delhi (2012).
3. Yadav, J. B., *Advanced Practical Physical Chemistry*, 33rd Ed., Goel Publishing House, New Delhi (2013).
4. Das, R. C.; Behera, B., *Experimental Physical Chemistry*, McGraw Hill Education (India), New Delhi (1984).

Literature Survey (5 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.

Project Work (10 Credit)

- Project work would be in lieu of Advanced Inorganic Chemistry Laboratory and Literature Survey.
- 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).

OPEN ELECTIVE COURSES

SEMESTER III

CHEO 541 OPEN ELECTIVE: Bioanalytical and Medicinal Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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: Spectroscopy 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. Prodrugs 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. Negi, A. S.; Anand, S. C., *Physical Chemistry*, 2nd Ed., New Age International Publishing, New Delhi (2014).
2. Harvey, D., *Modern Analytical Chemistry,* McGraw-Hill Higher Education (2000).
3. Metzler, D. E., *Biochemistry: The Chemical Reactions of Living Cells*, 2nd Ed., Academic Press (2003).
4. Colegate, S. M.; Molyneux, R. J. (Eds.), *Bioactive Natural Products: Detection, Isolation and Structural Determination,* 2nd Ed., CRC Press, Boca Raton (2008).

Further Reading

1. Mann, J.; Davidson, R. S.; Hobbs, J. B.; Banthrope, D. V., Harborne, J. B. *Natural Products, their Chemistry and Biological Significance*, Prentice Hall (1994).

SEMESTER III

CHEO 542 OPEN ELECTIVE: Applications of Molecular Spectroscopy

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

UNIT I: Applications of UV-Visible, IR 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 inorganic and coordination compounds.

UNIT II: Magnetic Resonance 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.
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: Mössbauer and NQR Spectroscopy
Mössbauer Spectroscopy: Basic principles, Doppler shift, recoil energy, isomer shift and interpretation. Quadrupole coupling. Applications to the studies of (a) bonding and structures of Fe^{2+} and Fe^{3+} compounds (b) metal carbonyls, (c) Sn^{2+} and Sn^{4+} compounds and (d) Iodine.
NQR Spectroscopy: Basic principles, electric field gradient (EFG), asymmetry parameter, effect of magnetic field. Application of NQR in transition metal complexes.

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. Application to organometallic compounds.

Recommended Books

1. Lampman, G. M.; Pavia, D. L.; Kriz, G. S.; Vyvyan, J.R., *Introduction to Spectroscopy*, 4th Ed., Cengage Learning India, New Delhi (2012).
2. Banwell C. N.; McCash, E. M., *Fundamentals of Molecular Spectroscopy*, 4th Ed., Tata McGraw Hill, New Delhi (2011).
3. Drago, R. S., *Physical Methods for Chemists*, 2nd Ed., Saunders College Publishing, Florida (1999).

4. Dyer, J. R., *Applications of Spectroscopy of Organic Compounds*, PHI Learning, New Delhi (2004).
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., John Wiley & Sons, New Jersey (2009).
2. Nakamoto, K., *Infrared and Raman Spectra of Inorganic and Coordination compounds*, *Part B: Applications in Coordination, Organometallic, and Bioinorganic Chemistry*, 6th Ed., John Wiley & Sons, New Jersey (2009).
3. Gunther, H., *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, 2nd Ed., Wiley India, New Delhi (1995).
4. Silverstein, R. M.; Webster, F. X., *Spectrometric Identification of Organic Compounds*, 6th Ed., Wiley India, New Delhi (2005).
5. William D. H.; Fleming, I., *Spectroscopic Methods in Organic Chemistry*, 6th Ed., McGraw Hill Education (India), New Delhi (2011).
6. Aruldas, G., *Molecular Structure and Spectroscopy*, 2nd Ed., PHI Learning, New Delhi (2007).

SEMESTER III

CHEO 543 OPEN ELECTIVE: Environmental and Green Chemistry

4 Credit 40 Contact Hours
Total Marks: 100 (Internal 20 + End Semester Exam 80)

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, 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*, 3rd Ed., Oxford University Press, New Delhi (2011).
2. Anastas, P. T.; Warner, J. C., *Green Chemistry: Theory and Practice*, Oxford University Press, New Delhi (2008).

Further Reading

1. Clark, J. H.; McQuarrie, D., *Handbook of Green Chemistry and Technology*, 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*, Anamaya Publishers, New Delhi (2006).