MATA GUJRI COLLEGE

FATEHGARH SAHIB

(AN AUTONOMOUS COLLEGE)

Masters in Science (Chemistry)

Programme Code: MSCHE

(Academic Year 2023-24)

PROGRAMME BROCHURE

(As approved by Academic Council)

M.Sc. Chemistry Revised Syllabus as per UGC Guidelines under CBCS (Choice Based Credit System)
Recommended by Board of Studies on 09.05.2023 and Approved by Academic Council

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ORDINANCES

MASTER OF SCIENCE (CHEMISTRY) EXAMINATIONS
(SEMESTER SYSTEM)

1. The examination for the degree of Master of Science (Chemistry) shall be held in two parts to be called Master of Science (Chemistry)Part-I and Master of Science (Chemistry)Part-II. Each part shall consist of two semesters viz. Semester 1st and 2nd in Part-I and Semester 3rd and 4th in Part-II. The examination shall be held in the months of November/December for 1st and 3rd Semester and April/May for 2nd and 4th Semester or on such other dates as may be fixed by the College. The amount of admission fee to be paid by a candidate per semester for the external examinations shall be as prescribed by the college from time to time.

2. M.Sc. (Chemistry)-I shall be open to a candidate who has passed B.Sc. Medical/Non-Medical, B.Sc. (Bio-Tech.) with Chemistry as an elective subject, B.Sc. Hons. (Chemistry) with at least 50% marks in the aggregate from Punjabi University, Patiala or any other University recognized as equivalent thereto by the Academic Council. M.Sc. (Chemistry)-II shall be open to any person who has passed M.Sc. (Chemistry)-I examination or has cleared at least 50% papers prescribed for first and second semester of M.Sc. (Chemistry) Programme.

   a) The Assessment in each semester of M.Sc. Programme will be 30% internal and 70% external for each theory paper. The result of the Internal Assessment shall be conveyed to the students/examination branch by the Head of the Concerned Department
   b) The internal assessment (Total marks 30) will be based on all or some of the following:
      - Mid Semester Tests 15 Marks (Two tests in each semester will be held and best of two will be taken for internal assessment)
      - Attendance 8 Marks
      - Assignments/reports/projects/Seminar 7 Marks

Note: If a case comes to notice of the Director-Principal, where the marks awarded by the Teacher are on a very Higher/Lower side, the award will be moderated by the following committee.

   i) Dean Academics of the College.
   ii) Dean of Faculty concerned.
   iii) Head of the Department concerned.

   If considered necessary, a member can be appointed by the Director-Principal on the recommendations of the Head, Chemistry Department of the college.

   There will be no internal assessment in a practical paper.

c) For a candidate who fails in a theory paper(s) the internal assessment examination for that paper will be carried over and the supplementary examination will, therefore, consist of only an external examination.

3. Minimum number of marks required to pass each semester examination will be 35% for each paper and 35% in the aggregate of the semester examination; 35% in practical papers. The candidate shall also be entitled to grace marks as admissible under the general ordinance relating to the 'Award of Grace Marks'.
4. The syllabus for the session shall be such as prescribed by the college and passed by members of Board of studies.
5. M.Sc. Chemistry examination is open only to a candidate who satisfies the following requirements:
   a) Has been on the rolls of the College throughout the Semester term preceding the examination.
   b) Of having good moral character.
   c) Of having attended not less than 75% lectures delivered to that class in each paper as well as 75% of the laboratory work, seminars etc. separately. Provided that a deficiency in attendances may be condoned for special reasons, as per the College rules.
6. The medium of instruction and examination shall be English.
7. Subject to completion of attendance requirement, there will be no condition of passing papers for promotion from odd semester to even semester in an Academic Session. A candidate placed under reappear in any paper, will be allowed two chances to clear the reappear, which should be availed within consecutive two years/chances i.e., to pass in a paper the candidate will have a total of three chances, one as regular student and two as reappear candidate.
8. The examination of reappear papers of odd semester will be held with regular examination of the odd semester and reappear examination of the even semester will be held with regular examination of even semester. But if a candidate is placed under reappear in the last semester of the Programme, the candidate will be provided a chance to pass the reappear with the examination of the next semester, provided their reappear of lower semester does not go beyond next semester. In case a candidate fails within the prescribed period, as aforesaid, the candidate shall be declared fail. Such a candidate may, however, seek fresh admission to the first semester on merit with the new applicants. It is understood that a 'reappear' or 'failed' candidate/s shall be allowed to take the examination in papers not

cleared by them according to the date sheets of the semester examinations in which such papers may be adjusted. After completing two years of studies (i.e., four semester Programme), the candidate shall not be admitted to any semester of the same Programme and will not have any privileges of a regular student. In case the student has one reappear in any of three semesters, then the student can give the reappear exam in the fourth semester by depositing the prescribed fees.

9. Viva Voce/ Practical examination shall be conducted by a Committee consisting of the following:
   i) One external examiner, ii) One internal examiner.
10. As soon as possible after the completion of each semester, the Registrar shall publish a list of successful candidates showing their result. Each candidate shall be supplied with a card containing his/her details of marks. Priorly, the list of successful candidates on the completion of M.Sc. Chemistry Programme shall be arranged in three divisions as follows; Successful candidates who obtain 60% or more of the aggregate number of marks in Part-I and Part-II examinations taken together, shall be placed in **first division**, those who obtain 50% marks or more but less than 60% shall be placed in the **second division** and those who obtain less than 50% and more than 35% shall be placed in the **third division**. Successful candidates who obtain 75% or more marks in the aggregate will be placed in the "**First Division with Distinction**".

In the adopted "Choice Based Credit system" pattern the above-mentioned pass % criterion has been revised to that of letter grade as given in the table, highlighted below. Each letter grade indicates the level of performance in the Programme and has a grade point for the purpose of computing the "Cumulative Grade Point Average" (CGPA) as given below.

Letter Grade	Marks	Grade points
O: Outstanding	91-100	10
A+: Excellent	81-90	9
A: very Good	71-80	8
B+: Good	61-70	7
B: Above Average	51-60	6

C: Average	41-50	5
P: Fair	35-40	4
F: Fail 0		0
D: Detained		0

11. *A candidate who has passed M.Sc. Chemistry examination from this college shall have one chance, within a period of two years, after passing the examination, to improve his division in a maximum of 1/3rd of total theory papers offered in both M.Sc. I & II examinations. The candidates shall also be entitled to grace marks as admissible under the ordinance relating to grace marks.
12. M.Sc. programme consists of several courses. The term 'Course' is applied to indicate a logical part of the subject matter of the programme and is invariably equivalent to the subject matter of a "paper" in the conventional sense.
    a) The specializations offered for the Programme are Inorganic, Organic and Physical which will be offered to candidates at the end of MSc. Part-I.
    b) The candidates are required to give their preference order for specialization.
    c) Specialization will be offered on merit basis made by average of B.Sc. and M.Sc. Semester-I marks.
    d) A minimum of passing marks will be given to candidates who have reappears for the purpose of calculation of their merit.
    e) The specialization opted once is for both Semesters III and IV courses and cannot be changed after Semester III.

**Note: Out of papers taken up the candidate will be given the benefit of increase in marks, where the marks have increased in Paper/Papers.*

Post Graduate Programme in Chemistry

PROGRAM EDUCATIONAL OBJECTIVES (PEOs)

The Postgraduates of the M.Sc. Chemistry programme are expected to:

PEO1: Acquire competencies and skills which can help them succeed in the chemistry related professions in academics, research, or industry.

PEO2: Analyse and solve complex chemical problems of relevance to the society through application of acquired skills and competencies.

PEO3: Demonstrate professional excellence, leadership qualities and contribute towards the development of their communities and society.

PEO4: Use scientific methods to approach and solve real life problems.

PEO5: Demonstrate moral values and professional ethics in their chosen careers and personal life.

PROGRAMME OUTCOMES (POs)

On successful completion of the M.Sc. chemistry programme, the students will be able to

PO1: Demonstrate an in-depth understanding of the scientific concepts, principles and processes related to chemistry and allied fields.

PO2: Design and perform experiments in a laboratory, handle scientific instruments and draw meaningful conclusions from the results obtained.

PO3: Communicate clearly scientific and technical information in written and oral manner.

PO4: Develop sense of enquiry, rational thinking, and scientific approach.

PO5: Work effectively as part of a team in a laboratory, industry, or some project.

PO6: Undertake discipline specific competitive exams conducted by service commissions and national agencies.

PO7: Pursue advanced studies or research in the chemistry related fields.

PO8: Work as professionals in educational institutes or chemical, pharmaceutical related industries.

PROGRAMME SPECIFIC OUTCOMES (PSOs)

On completion of the M.Sc. Chemistry programme, the students will be able to:

PSO1: Demonstrate in-depth knowledge and understanding about chemical concepts, principles, and processes in all the major areas of chemistry (analytical, inorganic, organic and physical), and its related fields.

PSO2: Demonstrate skills relating to chemical synthesis, identification, separation and analysis of metal ions and other inorganic/organic compounds useful for research and employment in academia and industry such as pharmaceutical industry, chemical industry, consumer goods industry, food products industry, cosmetics industry, and other related industries.

PSO3: Use chemical techniques of qualitative and quantitative analysis including instrumental analysis such as IR, NMR, and other spectroscopic techniques in the identification of inorganic and organic compounds at semi-micro level.

PSO4: Apply standard methodology to find solutions to problems in chemistry and its allied fields and appreciate the application of chemistry in environmental and social contexts.

Programme Structure

The Master of Science in Chemistry Programme is a Two-Year Full-Time Programme consisting of four semesters, to be known as Semester I, Semester II, Semester III and Semester IV.

Part I	First Year	Semester I	Semester II
Part II	Second Year	Semester III	Semester IV

Programme Structure

Semester	**Core courses**			**Discipline Specific Electives**			**Total Credits**
	No. of Theory + Practical Papers	Credits (L+P)	Total credits	No. of Theory + Practical Papers	Credits (L+P)	Total Credits	
I	4+2	20+7.5	27.5	0	0	0	27.5
II	4+2	20+7.5	27.5	0	0	0	27.5
III	3+1	15+3.75	18.75	1+1	5+3.75	8.75	27.5
IV	3+1	15+3.75	18.75	1+1	5+5.75	10.75	29.5
Total Credits for the programme 112							

Semester-wise Course Details

SEMESTER I				
Number of core courses	Six (4 Theory + 2 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Core Course 1	**5**	**0**	**0**	**5**
Core Course 2	**5**	**0**	**0**	**5**
Core Course 3	**5**	**0**	**0**	**5**
Core Course 4	**5**	**0**	**0**	**5**
Core Course 5	**0**	**3.75**	**0**	**3.75**
Core Course 6	**0**	**3.75**	**0**	**3.75**
Total Credits in Semester I	**27.5**			

SEMESTER II				
Number of core courses	Six (4 Theory + 2 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Core Course 7	**5**	**0**	**0**	**5**
Core Course 8	**5**	**0**	**0**	**5**
Core Course 9	**5**	**0**	**0**	**5**
Core Course 10	**5**	**0**	**0**	**5**
Core Course 11	**0**	**3.75**	**0**	**3.75**
Core Course 12	**0**	**3.75**	**0**	**3.75**
Total Credits in Semester II	**27.5**			

SEMESTER III				
Number of core courses	Six (4 Theory + 2 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Core Course 13	**5**	**0**	**0**	**5**
Core Course 14	**5**	**0**	**0**	**5**
Core Course 15	**5**	**0**	**0**	**5**
Core Course 16	**0**	**3.75**	**0**	**3.75**
Number of Discipline Specific Elective Courses	**2**			
Discipline Specific Elective 1	**5**	**0**	**0**	**5**
Discipline Specific Elective 2	**0**	**3.75**	**0**	**3.75**
Total Credits in Semester III	**27.5**			

SEMESTER IV				
Number of core courses	Six (4 Theory + 2 Practical)			
	Credits in each course			
	Theory	Practical	Tutorial	Total
Core Course 18	**5**	**0**	**0**	**5**
Core Course 19	**5**	**0**	**0**	**5**
Core Course 20	**5**	**0**	**0**	**5**
Core Course 21	**0**	**3.75**	**0**	**3.75**
Number of Discipline Specific Elective Courses	**3**			
Discipline Specific Elective 3	**5**	**0**	**0**	**5**
Discipline Specific Elective 4	**0**	**3.75**	**0**	**3.75**
Industrial Training	**0**	**2**	**0**	**2**
Total Credits in Semester IV	**29.5**			

Total credits of the programme = 27.5 + 27.5 + 27.5+ 29.5 = 112

Scheme of Programme M.Sc. Chemistry Part I (Semester I and II)

Course Code	Title of Paper	Credits LTP	No. of Lectures	Max. Marks (External + Internal) Pass Percentage 35%	Duration of Paper
		SEMESTER-I			
MSCHE 101	Inorganic Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 102	Organic Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 103	Physical Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 104	Analytical Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 105	Inorganic Chemistry Practicals-I	0 0 3.75	100	100	6 Hrs.
MSCHE 106	Analytical and Physical Chemistry Practicals	0 0 3.75	100	100	6 Hrs.
		SEMESTER-II			
MSCHE 201	Inorganic Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 202	Organic Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 203	Physical Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 204	Applications of Molecular Spectroscopy	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 205	Organic Chemistry Practicals-I	0 0 3.75	100	100	6 Hrs.
MSCHE 206	Physical Chemistry Practicals-I	0 0 3.75	100	100	6 Hrs.

Scheme of Programme M.Sc. Chemistry Part II (Semester III and IV)

SEMESTER III					
Course Code	**Title of Paper**	**Credits L T P**	**No. of Lectures**	**Max. Marks (External + Internal) Pass Percentage 35%**	**Hours/week**
MSCHE 301	Reaction Mechanisms of Transition Metal Complexes	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 302	Photochemistry and Pericyclic reactions	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 303	Advanced Physical Chemistry-I	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 304	Chemistry Practicals-I	0 0 3.75	100	100	6 Hrs.
Discipline Specific Electives					
MSCHE 311	Inorganic Spectroscopy	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 312	Inorganic Chemistry Practicals-II	0 0 3.75	100	100	6 Hrs.
MSCHE 321	Heterocyclic Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 322	Organic Chemistry Practicals-II	0 0 3.75	100	100	6 Hrs.
MSCHE 331	Chemical Thermodynamics	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 332	Physical Chemistry Practicals-II	0 0 3.75	100	100	6 Hrs.

SEMESTER IV					
Course Code	**Title of Paper**	**Credits L T P**	**No. of Lectures**	**Max. Marks (External + Internal) Pass Percentage 35%**	**Duration of Paper**
MSCHE 401	Chemistry of Organometallic Compounds	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 402	Name Reactions, Reagents and Rearrangements	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 403	Atmospheric Photochemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 404	Chemistry Practicals-II	0 0 3.75	100	100	6 Hrs.
MSCHE 411	Advanced Topics in Inorganic Chemistry	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 412	Inorganic Chemistry Practicals-III	0 0 3.75	100	100	6 Hrs.
MSCHE 421	Chemistry of Natural Products	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 422	Organic Chemistry Practicals-III	0 0 3.75	100	100	6 Hrs.
MSCHE 431	Advanced Physical Chemistry-II	5 0 0	60	100 (70+30)	3 Hrs.
MSCHE 432	Instrumental Physical Chemistry Practicals	0 0 3.75	100	100	6 Hrs.
MSCHE 405	Industrial Training and Report	0 0 2	50	50	

Note: In paper codes, first digit 1, 2, 3 and 4 stands for first, second, third and fourth semester respectively. The middle digit 0 stands for common paper, 1 for inorganic specialization, 2 for organic specialization and 3 for physical specialization. The last digit stands for specific paper. In second year, students must choose any one specialization out of Organic, Inorganic and Physical specializations. The students will study three common papers and one paper of a particular specialization in the third and fourth semester.

SEMESTER-WISE SYLLABUS
SEMESTER-I

MSCHE 101: INORGANIC CHEMISTRY

Maximum Marks: 100		L T P 5 0 0
Semester Examination: 70		Lectures: 60
Internal Assessment: 30	Time: 3hrs	Pass marks: 35%

COURSE OUTCOMES

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

CO1: Explain bonding, draw structures, and predict properties of important compounds of main group elements.

CO2: Explain the theoretical treatment of chemical bonding via valence bond theory and molecular orbital theory.

CO3: Determine splitting of d orbitals due to ligand field in different geometries and illustrate structural and thermodynamic consequences of crystal field splitting.

CO4: Find out term symbols arising out of various configurations and determine splitting of term symbols in weak crystal fields.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Main Group Elements:

Molecular, ionic and metallic hydrides; boron-nitrogen compounds: borazine, substituted borazines, and boron nitride; boron clusters: metal borides, structure and bonding of polyhedral boranes, closo, nido and arachno structures, structural study by NMR, Wade's rules, metalloboranes, carboranes, metallocarboranes; carbides, silicates, zeolites and clays.

Phosphorus-Nitrogen compounds: cyclo and linear phosphazenes; chemistry and bonding of sulphur-nitrogen compounds, iso and heteropoly acids and anions of Mo and W, interhalogen compounds, polyhalogen compounds, interhalogen cations, polyiodide anions. Noble gas compounds: synthesis, structure and reactions of xenon fluorides, xenon-oxygen compounds, compounds of krypton and radon.

Chemical Bonding:

Wave mechanical treatment of covalent bond, the variation principle, ground state energy of hydrogen atom, the secular equations, valence bond theory, concept of resonance, resonance energy, molecular orbital theory, LCAO principle, molecular orbital treatment of H_2^+ ion, construction of MO and VB wave functions, electron charge densities in molecular orbitals of H_2^+ ion, hybridization, wave functions for sp^3 hybrid orbitals, the three centered bond, Linnett's double quartet approach, the Pauli's exclusion principle.

UNIT II

Metal-Ligand Bonding in Coordination Complexes:

Crystal field theory, splitting of d-orbitals under the effect of octahedral, tetrahedral, tetragonal and square planar crystal fields, factors affecting the magnitude of crystal field splitting, the structural (ionic radii, Jahn-Teller effects) and thermodynamic effects (hydration and lattice energy) of crystal field splitting, the limitations of crystal field theory, the ligand field theory, evidences for metal-ligand overlap in complexes, molecular orbital theory for octahedral, tetrahedral and square planar complexes.

Atomic Spectroscopy:

Spin-spin coupling, orbital-orbital coupling, RS and J-J coupling schemes, determination of free ion terms for p^n and d^n configurations, determination of ground state terms-Hund's rule, hole formulism, and spin-orbit coupling.

Free Ions in Weak Ligand Fields:

The effect of octahedral fields on S, P, D and F terms (with help of the character table), splitting patterns of and G, H and I terms.

Books Recommended:

1. M.C. Day, J. Selbin, *Theoretical Inorganic Chemistry*.
2. J.D. Lee, *Concise Inorganic Chemistry*, 4th edition.
3. Shriver and Atkins, *Inorganic Chemistry*, 5th edition.
4. L. Miessler, D.A. Tarr, *Inorganic Chemistry*, 3rd edition.
5. F.A. Cotton, Wilkinson et al., *Advanced Inorganic Chemistry*, 3rd, 5th and 6th edition.
6. F. Basolo and R.C. Johnson, *Coordination Chemistry,* 1st edition.

MSCHE 102: ORGANIC CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

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

CO1: Reproduce structures and reactions of various reactive intermediates.
CO2: Predict and elucidate the mechanisms of certain organic reactions.
CO3: Appraise the nature of bonding in organic molecules.
CO4: Summarise various techniques used for determination of reaction mechanism.
CO5: Use the concept of aromaticity to know the aromatic nature of compounds.
CO6: Construct the correlation diagrams and apply various theories to the pericyclic reactions.
CO7: Write the mechanisms of elimination reactions and deduce their stereochemical outcomes.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Reactive Intermediates:

Carbocations: Generation, Structure, Stability, allylic and benzylic carbocations. Stereochemistry and reactions. Nonclassical carbocations, Phenonium ion, norbornyl system. Application of NMR spectroscopy in the detection of carbocations. Carbanions: Generation, structure, stability, stereochemistry, and general reactions. Carbenes: Formation, Structure, Singlet and Triplet carbene, Stereochemistry and reactions. Nitrenes: Formation, Structure Singlet and Triplet nitrene, Stereochemistry and reactions. Arynes: Formation, Structure, and reactions. Free radicals: Formation, Structure, Stability, Stereochemistry, and reactions.

Reactions of Free Radicals:

Polymerisation, Halogenation: Chlorination, Bromination by NBS, Iodination, Fluorination. Polar effects in halogenations. Addition reactions: Free radical addition of HBr, thiols and halogens. Auto-oxidation. Rearrangements.

Nature of Bonding in Organic Molecules:

Introduction to fullerenes, Aromaticity in benzenoid and non-benzenoid compounds, Alternant, and non-alternant hydrocarbons, Huckel's rule, Anti-aromaticity, Homoaromaticity, Annulenes. Bonding weaker than covalent: Addition compounds, Crown ether complexes and Cryptands, Inclusion compounds, Cyclodextrins, Catenanes and Rotaxanes.

Techniques used for Determination of Reaction Mechanism:

Use of optical, stereochemical and isotope techniques. Reaction studies from Identification of Products, Trapping of Intermediates, Crossover Experiments, Use of Catalyst, Use of isotopes in reaction mechanism studies in case of Favorskii, Claisen and Benzyne reactions.

UNIT-II

Pericyclic Reactions:

Molecular orbital symmetry, Frontier orbitals of ethylene; 1, 3-butadiene; 1, 3, 5 hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO & PMO approach. Electrocyclic reactions: Conrotatory and Disrotatory motions, 4n, 4n+2, and allyl systems. Cycloadditions: antarafacial and suprafacial additions, 4n, 4n+2 systems, 2+2 addition of ketenes; 1,3-dipolar cycloadditions and chelotropic reactions. Sigmatropic rearrangements: suprafacial and antarafacial shift of hydrogen, Sigmatropic shifts involving carbon moieties. 3, 3- and 5, 5- sigmatropic rearrangements. Claisen, Cope rearrangements.

Elimination Reactions:

E_2, E_1 and E_1cB mechanism, stereochemistry, product ratio, orientation of double bond, Hoffman's rule, Saytzeff's rule, Factors governing E_2 and E_1 mechanism. Mechanism and orientation in pyrolytic elimination reactions.

Cyclic Elimination:
Amine Oxide, Esters, Xanthates, Free radical elimination. Elimination versus substitution. Effect of solvent, Temperature, Nature of Base, Structure of Reactant.
Nucleophilic Aromatic Substitution:
Benzyne, Nucleophilic aromatic substitution, addition-elimination mechanism**.**

Books Recommended:

1. *Advanced Organic Chemistry-Reactions, Mechanism and structure*, Jerry March, John Wiley.
2. *Advanced Organic Chemistry,* F.A. Carey & R.J. Sundberg, Plenum.
3. *A guidebook to Mechanism in Organic Chemistry,* Peter Sykes, Longman.
4. *Structure and mechanism in Organic Chemistry*, C.K. Ingold, Cornell University Press.
5. *Organic Chemistry,* R.T. Morrison and R.N. Boyd, Prentice Hall.
6. *Modern Organic Reactions,* H.O. House, Benjamin.
7. *Reaction Mechanism in Organic Chemistry*, S.M. Mukherji & S.P. Singh. Macmillan.
8. *Highlights of Organic Chemistry*, *An Advanced Textbook,* W.J.L. Nobel.

Link for relevant e-resources

https://epgp.inflibnet.ac.in/Home/ViewSubject?catid=13G8VouhmrFfuhs6rkiyTA==
https://swayam.gov.in/

MSCHE 103: PHYSICAL CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

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

CO1: Explain about the interactions of electromagnetic radiation and matter and their applications in spectroscopy.

CO2: Illustrate the principles, instrumentation and important applications of Microwave, IR, Raman, UV, NMR, NQR, ESR, CD, ORD and Electronic spectroscopic techniques.

CO3: Analyze and interpret spectroscopic data collected by the methods discussed in the course.

CO4: Solve problems related to the structure, purity, and concentration of chemicals.

CO5: Interpret molecular structures by choosing suitable spectroscopic methods and corresponding data.

INSTRUCTIONS FOR THE PAPER-SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT- I

Introduction

Electromagnetic radiation, interaction of electromagnetic radiation with molecules and various types of spectra, Born Oppenheimer approximation, absorption and emission spectroscopy, difference between atomic and molecular spectroscopy, types of spectroscopies, selection rules, width, and intensities of spectral lines. importance of spectroscopy.

Microwave Spectroscopy

Introduction to microwave spectroscopy, theory of microwave spectroscopy, linear molecules, instrumentation, spherical top molecules, symmetric top molecules, asymmetric top molecules, stark effect, relative intensities of microwave spectroscopy, applications to microwave spectroscopy (structural determination of $XeOF_4$, OCS, C_6H_5CN, O_3, inversion spectrum of ammonia).

Infrared Spectroscopy

Theory of infrared spectroscopy, instrumentation, vibrational frequency, factors which influence vibrational frequency, selection rules, difference between microwave spectroscopy and infrared spectroscopy, applications to infrared spectroscopy to quantitative analysis, limitations of infrared spectroscopy.

Rotation Vibration Spectroscopy

Rotation vibration spectroscopy of diatomic molecules, and polyatomic molecules, P, Q, R branches.

Raman Spectroscopy

Quantum and classical theory of Raman effect, rotational Raman spectrum of diatomic molecules, rotational – vibrational Raman spectrum, resonance Raman spectrum, intensity of Raman peaks, structure determination from Raman and IR spectroscopy, applications of Raman spectroscopy in physical chemistry (ionic equilibria in solution, study of single crystals).

UNIT-II

Nuclear Magnetic Resonance (NMR)

Introduction to nuclear magnetic resonance, equivalent and non-equivalent protons, spin-spin coupling, coupling constants, number of signals, chemical shift, instrumentation, interpretation of NMR spectroscopy of ethyl bromide, isopropyl bromide, ethanol, ethanal, acetophenone, solvents used in NMR spectroscopy, limitations of NMR spectroscopy, NMR of paramagnetic compounds, magnetic resonance imaging (MRI). applications of NMR spectroscopy (structure determination of WF_6, SOF_6, HF_2^-, polythene, linkage isomerism, ligand isomerism).

Nuclear Quadrupole Resonance (NQR)

Introduction to NQR, theory of NQR, sample requirements, applications of NQR (nature of chemical bond, structural information about group III halides, study of charge transfer complexes, study of chloromethanes chloroacetyl chlorides, chlorides and disubstituted of benzenes).

Electron Spin Resonance (ESR)

Introduction to ESR, comparison between NMR and ESR, theory of ESR, choice and concentration of solvent, instrumentation, presentation of the ESR spectrum, hyperfine structure of the ESR spectrum, determination of g value, deviation of the g value, line width, Kramer's degeneracy and zero field splitting (ZFS), applications of ESR spectrum (study of free radicals, structural determination, reaction velocities and mechanism, biological systems, analytical applications).

Electronic Spectroscopy

Introduction to electronic spectroscopy (origin and theory), Frank Condon Principle, vibrational coarse structure of electronic spectra, Fortrat diagram, solvent effect, choice of solvent, electronic spectra of transition metal ions, charge transfer spectra.

Optical Rotatory Dispersion and Circular Dichroism

Theory of polarized light, optical activity and optically active molecules, instrumentation, optical rotatory dispersion (ORD), circular dichroism (CD), Cotton effect, Octant rule, applications of ORD (quantitative analysis, conformation studies, equilibrium studies) and CD (protein conformation, conformation of nucleic acid).

Books Recommended:

1. Molecular Spectroscopy, C.N. Banwell.
2. Molecular Spectroscopy, G.M. Barrow.
3. Atomic structure, chemical bonding including Molecular Spectroscopy. M. Chandra.
4. Organic Spectroscopy - Principle and applications, Jagmohan.
5. Physical Spectroscopy, Sham K Anand. & Gurdeep R. Chatwal.
6. Physical methods in Inorganic Chemistry, R. S Drago.
7. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish.

MSCHE 104: ANALYTICAL CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

After the completion of this course student will be able to:

CO1: Analyse different errors using statistical methods in chemical analysis.
CO2: Evaluate errors in chemical analysis through statistical treatment of data through F-test, T-test and Q-test.
CO3: Develop an insight into the practical methods for performing thermogravimetric analysis, potentiometric and conductometric titrations and their graph analysis.
CO4: Learn the concept of solvent extraction and apply it in metallic and organic compound extractions.
CO5: Adopt different chromatographic techniques for isolation of organic compounds.
CO6: Apply various methods for the synthesis of nanoparticles which is nowadays an emerging field of sciences.
CO7: Develop skills in problems solving, critical thinking and analytical reasoning.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT- I

Qualitative and Quantitative Aspects of Analysis

Sampling, evaluation of analytical data: Errors, accuracy and precision, methods of their expression, normal law of distribution, indeterminate errors, statistical test of data: F, Q, and T test, rejection of data, and confidence intervals, calibration curve, standard addition method, detection limit and detection range.

Thermo-Analytical Methods

Thermogravimetric analysis: Introduction, instrumentation, factors affecting thermogravimetric results, applications of thermogravimetry. Differential Thermal Analysis (DTA) and Differential Scanning Calorimetry (DSC) on-line analysis. Thermometric titrations Introduction theory and applications.

Electro-Analytical Methods

Polarography: D.C. and A.C. Polarography, pulse polarography, cyclic voltammetry, Linear Sweep Voltammetry (LSV) and Differential Pulse Voltammetry (DPV), qualitative and quantitative applications of polarography and cyclic voltammetry. Amperometric and biamperometric titrations.

Electrogravimetry: Current-voltage relationship during electrolysis, instrumentation, and applications of electrogravimetry.

Coulometry: Coulometric methods at constant current and constant electrode potential, coulometric titrations.

UNIT-II

Solvent Extraction

Distribution constant, distribution ratio and their importance in solvent extraction, synergistic extraction, extraction by solvation, ion pair formation, methods of extraction and their applications in analytical chemistry.

Chromatography

Thin layer chromatography (TLC): Introduction, principle and technique of TLC, High Performance Thin Layer Chromatography (HPTLC).

Liquid Chromatography: Introduction, types of liquid chromatography, mobile phase, sample injection and column design, column efficiency, Basic introduction to High Performance Liquid Chromatography (HPLC).

Gas Chromatography: Introduction, apparatus, and applications.

Characterization of Nanomaterials

Definition, historical perspective and effects of nanoscience and nanotechnology on various fields, Synthesis of nanoparticles by chemical routes, thermodynamics and kinetics of nucleation, growth of polyhedral particles by surface reaction, Ostwald ripening, size distribution and hydrodynamic size. Introduction to Characterization techniques: Transmission Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), Atomic Force Microscopy (AFM), Dynamic light scattering (DLS), XPS, and EDX.

Properties of nanostructured materials: Optical properties (Absorption, Emission and SPR); magnetic properties; chemical properties. Overview of applied chemistry of nanomaterials.

Books Recommended:

1. *A Textbook of Quantitative Inorganic Analysis:* Vogel, Arthur I: (Rev. by GH Jeffery and others) 5th Ed.
2. *Instrumental Methods of Analysis;* Willard, Hobert H. *et al*: 7th Ed. Wards worth Publishing Company, Belmont, California, USA, 1988.
3. *Analytical Chemistry*; Christian, Gary D; 6th Ed. New York- John Willy, 2004.
4. *Basic concept of Analytical Chemistry;* Khopkar, S.M.; New Age, International Publisher, 2009.
5. *Modern Polarographic methods in Analytical Chemistry,* A.M. Bend.
6. *Principles of Instrumental Analysis;* Skoog, D.A. Holler F.J. and Nieman, T.A. Thomson Asia Pvt. Ltd. Singapore.
7. *Instrumental Methods of Analysis;* D.A. Skoog.
8. *Nanotechnology, Fundamentals and Applications;* Manasi Karkare, I.K. International Publishing House Pvt. Ltd.
9. *A Textbook of Nanoscience and Nanotechnology;* T. Pradeep, Tata McGraw Hill.

MSCHE 105: INORGANIC CHEMISTRY PRACTICALS-I

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

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

CO1: Perform standardization of various reagents like $KMnO_4$, $K_2Cr_2O_7$, $Na_2S_2O_3$ and carry out oxidation-reduction titrations.

CO2: Perform precipitation titrations using $AgNO_3$.

CO3: Determine metals by complexometric titrations using EDTA.

CO4: Perform gravimetric/titrimetric determination of mixed metal ions.

CO5: Carry out synthesis of simple coordination compounds.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:

Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

PRACTICALS

1. Oxidation Reduction titrations:

a) Standardisation of $KMnO_4$ and determination of nitrites.
b) Standardization of $K_2Cr_2O_7$ and determination of Fe^{2+}.
c) Standardisation of $Na_2S_2O_3$ with KIO_3 and determination of I^-.

2. Precipitation Titrations:

a) Standardization of $AgNO_3$ by using adsorption indicator.

b) Standardization of thiocyanate solution and determination of chloride by Volhard method.

3. Complexometric Titrations:

a) Determination of Ca^{2+} in milk.
b) Determination of Al^{3+} by back titration.
c) Determination of Cu^{2+} and Ni^{2+} by using masking reagents.
d) Determination of total hardness of water by EDTA titration.

4. **Gravimetric/titrimetric determination of mixed ions:**

a) Copper-Nickel.
b) Iron-nickel.
c) Copper-Zinc.

5. **Preparation of following compounds**:

a) Preparation of tetraamminecopper(II)sulphate.
b) Preparation of hexamminecobalt(III)chloride.
c) Preparation of tris-thioureacopper(I)chloride.

Books recommended:

1. *Vogel's Quantitative chemical Analysis,* Pearson Education, 6th edition.
2. *Vogel's Qualitative Inorganic Analysis,* Pearson Education, 5th edition.
3. *Advanced Practical Inorganic Chemistry,* Gurdeep Raj, Krishna Prakashan.

MSCHE106: ANALYTICAL AND PHYSICAL CHEMISTRY PRACTICALS

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

On completion of the course students will be able to

CO1: Perform the practicals of analytical chemistry and able to know about direct titration, redox titration, adsorption indicator, complex reactions using EDTA.

CO2: Demonstrate the practicals refractometer and determine molar refractivity.

CO3: Able to calculate equilibrium constant by partition method.

CO4: Demonstrate the practicals of viscosity, surface tension and refractometer.

CO5: Develop various skills like observation, teamwork, scientific thinking.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:
Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

PRACTICALS:

1. To determine the percentage purity of given sample of KBr using adsorption indicator (Eosin).
2. To determine the strength of ascorbic acid in the given solution of vitamin C tablet by titrating against (a) standard I_2 solution (b) standard sodium thiosulphate solution.
3. To determine the amount of H_2O_2 in the given solution by titrating against (a) standard $KMnO_4$ solution (b) Standard sodium thiosulphate solution.

4. To determine the percentage purity of given sample of KI by titrating against standard KIO_3 solution.
5. To determine Zn^{2+}/Mg^{2+} by titrating against EDTA using Eriochrome Black T as an indicator.
6. To determine Nickel using murexide as indicator (direct titration).
7. To find out the equilibrium constant for the given reaction, $KI+I_2 = KI_3$ by partition method.
8. To determine the surface tension of homologous series of alcohols/ esters and alkane. Then determine the atomic parachors of C, H and O.
9. To compare the cleansing powers of two samples of detergents by surface tension method.
10. To determine the interfacial tension between two immiscible solvents (water -benzene, water-toluene) by surface tension method.
11. To determine the molecular weight of a given polymer by viscosity method.
12. To find out the molar refractivity of homologous series of alcohols and find out the atomic refractivities of C, H and O.

Books Recommended:

1. Advanced Physical Chemistry Experiments, Gurtu-Gurtu.
2. Senior Practical Physical Chemistry, B.D.Khosla V.C Garg & Adarsh Gulati.
3. Practical Physical Chemistry, B. Viswanathan & P.S Raghavan.
4. Practical Physical Chemistry, A.M. James and F. E. Prichard, Longman.
5. Practical Physical Chemistry, Alexander and Findley.
6. Advanced Practical Chemistry, Jagdamba Singh, R.K.P Singh, Jaya Singh.
7. Advanced Practical Chemistry, R. Mukhopadhyay and P. Chatterjee.
8. University Practical Chemistry, P.C. Kamboj.
9. Advance Practical Physical Chemistry, J. B.Yadav.
10. Textbook of Chemistry Practical, Bidhan Chandra Ray and Satyanarayan Das.

SEMESTER-II

MSCHE 201: INORGANIC CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

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

CO1: Determine symmetry point groups of molecules and list the symmetry elements, symmetry operations present in the group.
CO2: Construct character tables and apply character tables to determine hybridization of molecules and splitting of orbitals in different geometries.
CO3: Find out term symbols arising out of various configurations and determine splitting of these term symbols under ligand field.
CO4: Interpret electronic spectra of transition metal complexes.
CO5: Predict magnetic properties of transition metal complexes.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.
Note: Use of character tables and correlation table is allowed.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Symmetry and Group Theory:

The concept of group, order and classes of group, symmetry elements, symmetry operations and their matrix representation, multiplication tables, point group determination, determination of reducible and irreducible representations, construction of character tables for C_{2V} and C_{3V} point groups, application of group theory to chemical bonding, splitting of d-orbitals under the influence of octahedral symmetry, the directed valence for *Oh* and *Td* symmetry, use of character tables to determine which metal orbitals are used in σ and π bond formation in octahedral, tetrahedral and square planar complexes, molecular orbital energy level diagrams for octahedral, tetrahedral and square planar complexes showing σ and π bonding in transition metal complexes.

Free Ions in Medium and Strong Crystal Fields:

Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d^2 configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d^2 configuration in octahedral field, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams (d^2 and d^8 Octahedral).

UNIT-II

Electronic Spectra of Transition Metal Complexes:

Selection rules, band widths, band intensities, Symmetry considerations regarding selection rules and spectral intensities, vibronic coupling, vibronic polarization in centrosymmetric complexes and non-centrosymmetric complexes, polarization of electronically allowed transitions,, nature of electronic transitions in complexes, spectra of aqueous solutions of hexaaquometal complexes $[M(H_2O)_6]^{n+}$, discussion of electronic spectra of octahedral d^1–d^9 metal ions, calculation of 10Dq and B with use of Orgel and Tanabe Sugano diagrams, spectrochemical and nephelauxetic series, charge transfer spectra.

Magnetic Properties of Transition Metal Complexes:

Magnetochemistry: Origin of Magnetic moment, Magnetic susceptibility (diamagnetic, paramagnetic), spin only moment, Russell Saunder‘s coupling, quenching of orbital angular

moment, orbital contribution to a magnetic moment, magnetic moments from magnetic susceptibilities, temperature dependence of magnetic susceptibility, Factors determining paramagnetism, application of magnetochemistry in co- ordination chemistry in spin free and spin paired octahedral and tetrahedral complexes, Van Vlecks formula for magnetic susceptibility.

Books Recommended:

1. F.A. Cotton, *Chemical Applications of Group Theory.*
2. G. Davidson, *Introductory Group Theory for Chemists.*
3. B.N. Figgis, *Introduction to Ligand Field.*
4. A.B.P. Lever, *Inorganic Electronic Spectroscopy.*
5. R.S. Drago, *Physical Method in Chemistry.*
6. A. Earnshaw, *Introduction to Magnetochemistry*.

MSCHE 202: ORGANIC CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

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

CO1: Apply stereochemical aspects to reaction mechanisms and learn methods of racemisation and resolution.

CO2: Recognize stereochemistry and be able to apply the Cahn-Ingold-Prelog system to designation of stereochemistry (E/Z, R/S).

CO3: Demonstrate stereochemistry and draw various possible conformations of organic compounds.

CO4: Elaborate the concepts related to Conformational Isomerism and geometrical isomerism.

CO5: Recognize mechanistic and stereochemical aspects of addition reactions to carbon-carbon multiple and carbon-hetero multiple bonds.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Stereochemistry:

Stereoisomerism: Introduction and different types of stereoisomerism. Fisher, Newman and Sawhorse representations for organic compounds and their interconversions. Optical isomerism: Requirement for a compound to be optically active, compounds with one asymmetric centre. Dissymmetry as a cause of optical activity Molecules with two asymmetric centres. Racemic modification. Racemisation: Thermal, anionic, cationic, free radical, epimerization, Mutarotation, Racemic compounds mixtures and solid solutions.

Methods of resolution of acids, bases, amino acids, alcohols, aldehydes, and ketones. Absolute and relative configuration, Different systems of notation. Asymmetric induction, Methods of determining the configuration: Cram's Rule and Prelog's Rule.

Conformational Isomerism:

Meaning of conformation. Conformation and reactivity in alicyclic compounds. Conformational effects on stability and reactivity. Ionic elimination. Intramolecular rearrangement, Neighbouring group participation. Pyrolysis of acetates xanthates and amine oxides.

Relation of conformation to reactivity, Optical isomerism due to restricted rotation in biphenyls, allenes, alkylidenes and spiranes and determination of their absolute configuration.

Conformational studies in cycloalkanes, mono and disubstituted cycloalkanes, stability, and reactivity. Studies in fused systems: Decalins and Perhydrophenanthrenes.

Geometrical Isomerism:

Nomenclature (E & Z) Nature of geometrical isomerism. Curtin-Hammett Principle. Study of Physical properties of the isomers, Relative stability, and interconversion of Geometrical isomers.

UNIT-II

Addition to Carbon-Carbon Multiple Bond:

Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles, and free radicals. Regioselectivity and Chemoselectivity. Orientations and reactivity. Addition to cyclopropane ring. Hydrogenation of double bond and triple bond and aromatic rings. Hydroboration, Michael reaction, Sharpless Asymmetric Epoxidation.

Addition to Carbon-Hetero Multiple Bond:

Mechanism of Metal hydrides reduction of carbonyl compounds and other functional groups, Dissolving metal reductions and conjugated systems.

Wolf-Kishner reduction, Clemmenson reduction, Meerwein-Ponndorf-Verley reduction, Wittig's reaction, Addition of Grignard's reagent, Organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds.
Mechanism of condensation reactions involving enolates: Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

Books Recommended:

1. *Stereochemistry of Carbon compounds,* Ernest L.Eliel, Tata McGraw Hill.
2. *Stereochemistry of Organic Compounds*, D. Nasipuri, New Age International.
3. *Stereochemistry of Organic Compounds,* P.S. Kalsi, New Age International.
4. *Modern Organic Reactions,* H.O. House, Benjamin.
5. *Organic Chemistry,* Clayden, J.; Greeves, N.; Warren, S.; Wothers, P.; Oxford University Press.
6. *Advanced Organic Chemistry, Reactions, Mechanism and structure*, Jerry March, John Wiley.

MSCHE 203: PHYSICAL CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

On the completion of the course, students will be able to:
On the completion of the course the students will be able to:
CO1: Know about absorption, adsorption, monolayer and multimolecular adsorption and theories related to them.
CO2: Compare the heterogeneous and homogeneous catalysts.
CO3: Compare strong and weak chemical interactions and comment on their role in physisorption and chemisorption.
CO4: Explain adsorption isotherms and how selected isotherms could be used for measurement of surface area of materials. Examination of surfaces using different spectroscopic technique
CO5: Elaborate step-growth and chain growth polymerization, with respect to mechanism and kinetics. Distinguish between absolute and relative methods for molecular weight determination using osmotic pressure, viscometry, light scattering, sedimentation method etc.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

Dr. Ashok Kumar Malik | Dr. Manmohan Chhibber | Dr. Narinder Singh | Dr. Kamalpreet Kaur | Ms. Simrat Kaur | Dr. Kiran

Mr. Tejinder Singh | Mr. Punit Bhardwaj | Dr. Kuldeep Kaur | Ms. Seema Maheshwari | Dr. Manpreet Kaur | Dr. Poonam Patyar

UNIT-I

Surface Chemistry I

Adsorption, absorption, gas solid interface, physio sorption, chemisorption, cumulative and depletive chemisorption, Elovich equation, heat and activation energy of adsorption, factors on which adsorption depends, difference between chemical and physical adsorption.

Unimolecular adsorption isotherms: Freundlich and Langmuir adsorption isotherm, Tempkin isotherm.

Multilayer adsorption isotherms: BET theory and Harkins-Jura theory.

Statistical treatment of Langmuir adsorption isotherm, Nature and significance of constant c in BET equation, Thermodynamics of insoluble surface films on liquids, adsorption from solutions on solids, determination of surface area of adsorption by BET method, Gibbs adsorption equation and its verification, two-dimensional perfect gas equation, Gibb's and Langmuir equation, surface films.

Surface Chemistry II

Kinetics of heterogeneous reaction at solid surfaces, Kinetics and mechanisms of surface reactions, unimolecular and bimolecular surface reactions, retardation of reactants and products, activation energies of surface reactions, , absolute rate theory of heterogeneous reaction .

Examinations of surfaces using spectroscopic techniques: Electron spectroscopy for chemical analysis (ESCA), Photo electron spectroscopy (PES), Auger electron spectroscopy (AES), Scanning tunneling microscopy (STM), and low energy electron diffraction (LEED).

Properties of surface phase, surface active substances, surface inactive substances, surface pressure, micelles, wetting, surface tension, interfacial tension, detergency, electrokinetic effects, Important applications of surface chemistry.

UNIT-II

Polymer Chemistry

Introduction, classification of polymers, Types of stereoisomerism of polymers, properties of stereoregular polymers, kinetics of polymers, thermodynamics of polymer solutions (Flory-Huggins Theory), structure dynamics, composition and polymerization mechanism, physical states, determinants of polymer crystallinity, degree of polymerization, chain length.

Step polymerization

Reactivity of functional groups, basis for analysis of polymerization, kinetics of step polymerization, self-catalysed polymerization, external catalysis of polymerization, step polymerization other than poly esterification, non-equivalent of functional groups in polyfunctional reagents.

Radical Chain Polymerization

Overall kinetics of chain polymerization, initiation, thermal decomposition of initiators, types of initiators, kinetics of initiation and polymerization, dependence of polymerization rate on monomer, photochemical initiation, initiation by ionizing radiation, pure thermal radiation, redox initiation.

Molecular weight of polymers

Number average molecular weight, weight average molecular weight, poly dispersed index (PDI), Molecular weight determination by osmotic pressure method, diffusion method, light scattering method, sedimentation method, and viscosity method.

Books Recommended:

1. *Principles of polymerization, George Odian.*
2. *Principles of polymer chemistry, Paul J. Flory.*
3. *Textbook of physical chemistry, Glasstone.*
4. *Text book of physical chemistry, G.M.Barrow.*
5. *Surface chemistry, A. Singh and R. Singh.*
6. *Textbook of physical chemistry of surfaces, Arthur W. Adamson.*
7. *Surface c*hemistry, Elaine M. Mc Cash.

MSCHE 204: Applications of Molecular Spectroscopy

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

After the completion of this course student will be able to

CO1: Explain basic principles of various spectroscopic techniques.
CO2: Make use of various spectroscopic methods used for the characterization/identification of compounds.
CO3: Solve the problems related to structure of compounds by analysing the spectral data.
CO4: Apply the understanding to the identification of compounds.
CO5: Determine the *λmax* for various compounds.
CO6: List and explain factors affecting the measurements in various spectroscopic techniques.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Ultraviolet and Visible Spectroscopy

Principle of UV spectroscopy, Colour and light absorption, the chromophore concept, theory of electronic spectroscopy, orbitals involved and electronic transition. Effect of solvent and

conjugation on λ_{max}. Woodward Fieser, Fieser-kuhn and Nielsen's rules. Spectral correlation with structure; Conjugated dienes and polyenes; α, β-unsaturated carbonyl compounds; Benzene, substituted benzene and polynuclear aromatic hydrocarbons. Stereochemical factors in electronic spectroscopy; biphenyls and binaphthyls, cis and trans isomers, angular distortion, cross conjugation, and steric inhibition of resonance.

Infrared Spectroscopy

Principle of IR spectroscopy, Molecular vibrations, and modes of vibrations. Factors influencing vibrational frequencies; vibrational coupling, hydrogen bonding, conjugation, inductive, mesomeric (resonance), field effects and bond angles. Applications to identify functional groups; Aliphatic, aromatic and aralkyl hydrocarbons, alcohols, phenols, and ethers; aldehydes, ketones, carboxylic acid and ester, amines, amides, alkyl halides, aryl halides and aralkyl halides. Heteroaromatic compounds (pyrrole, furan and thiophene) and amino acids**.**

Mass Spectrometry

Introduction, Mass spectra and metastable ion peak. Determination of molecular formula and recognition of molecular ion peak and the Nitrogen rule. Molecular formula and index of hydrogen deficiency. General rules of fragmentation and the McLafferty rearrangement. Fragmentations associated with functional groups: Aliphatic, aromatic, aralkyl hydrocarbons, alcohols, phenols and ethers, aldehydes, ketones, carboxylic acids, esters, amines and amides, alkyl halides, aryl halides and aralkyl halides. Heteroatomic compounds (pyrrole, furan, thiophene) and amino acids.

UNIT-II

Nuclear Magnetic Resonance Spectroscopy

Proton Magnetic Resonance Spectroscopy, Nuclear spin resonance, Chemical shift and its measurement, Relaxation processes, Factors influencing chemical shift, shielding and deshielding and anisotropic effects, Effect of restricted rotation, concentration, temperature and hydrogen bonding, Spin-Spin coupling (simple and complex), Mechanism of coupling. Coupling constants, geminal coupling, vicinal coupling, virtual and long-range coupling, Factors influencing geminal and vicinal coupling, chemical equivalence and magnetic equivalence of protons, non-first order spectra, Simplification of complex PMR spectra: increasing strength, spin decoupling or double resonance and the use of chemical shift reagents. Variable temperature NMR spectroscopy: Introduction and applications.

^{13}C-NMR Spectroscopy

Natural abundance of ^{13}C, resolution and multiplicity. The FT mode and rf pulse. Use of proton coupled, proton decoupled and off-resonance decoupling techniques, Deuterium substitution and chemical shift equivalence in peak assignments. ^{13}C chemical shift; effect of substituents on chemical shift position of alkanes, alkenes, alkynes, and benzene. Spin-Spin coupling and ^{13}C-^{1}H coupling constants.

Structure Elucidation with the use of one or more of spectroscopic data of molecules.

Books Recommended:

1. *Organic Spectroscopy,* William Kemp, Macmillan, Hampshire, UK, 1991.
2. *Spectroscopic methods in Organic Chemistry,* D.H. William and I. Fleming, Tata Mac Graw-Hill Publishing company Ltd. New Delhi, India, 1991.
3. *Spectrometric Identification of Organic Compounds,* R.M. Silverstein, G. C. Bassler and
4. F.C Morill, 5th Edition, John Wiley and Sons Inc., USA, 1991.
5. *Introduction to spectroscopy,* Donald L. Pavia.
6. *Elementary Organic Spectroscopy; Principles and Chemical Applications,* Y.R. Sharma.
7. *Organic Structures from Spectra*, L. D. Field, S. Sternhell, J. R. Kalman.

MSCHE 205: ORGANIC CHEMISTRY PRACTICALS-I

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

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

CO1: Separate and purify an organic mixture by chemical/solvent separation methods.

CO2: Prepare organic compounds via two step synthetic sequences.

CO3: Apply methods employed for reactions like oxidation, condensation, substitution, and heterocyclic ring formation etc.

CO4: Monitor the progress of the reaction by chromatographic and spectral technique (FTIR).

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:

Experiment I: 35 marks

Experiment II: 35 marks

Viva-Voce: 20 marks

Practical Record Book: 10 marks

PRACTICALS

Qualitative Organic Analysis:

Separation and Purification of components of binary mixture (solid/solid, solid/liquid, liquid/liquid) based on solubility behaviour and solvent extraction and their identification and conformation by chemical tests and preparation of suitable derivative.

Organic Synthesis:

1. Benzoylation: Hippuric acid
2. Oxidation: Adipic acid/*p*-Nitrobenzoic acid
3. Aldol condensation: Dibenzalacetone/Cinnamic acid
4. Sandmeyer's reaction: *p*-Chlorotoluene
5. Benzfused Heterocycles: Benzimidazole

6. Cannizzaro's reaction: *p*-Chlorobenzaldehyde as substrate
7. Friedel Crafts reaction: *β*-Benzoylpropionic acid
8. Aromatic electrophilic Substitution: *p*-Nitroaniline/*p*-Iodoaniline

The products may be characterized by spectral techniques and checking the purity of prepared compounds by Thin Layer Chromatography.

Note: *Subject to the availability of Instrument/Chemicals, the experiments can be substituted by alternate experiments.*

Books Recommended:

1. *Vogel's Textbook of Practical Organic Chemistry*, 5th Edition ELBS (Longman), 1996.
2. *Practical Organic Chemistry,* F.G. Mann and B.C. Saunders, 5th Edition, Orient Longman Limited, 1986.

MSCHE 206: PHYSICAL CHEMISTRY PRACTICALS-I

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:

COURSE OUTCOMES

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

CO1: Illustrate the instrumentation and important applications of UV-Visible spectrophotometric/colorimeter and polarimeters. techniques.

CO2: Perform complexometric titrations with UV-visible spectrophotometer.

CO3: Operate polarimeter and able to determine specific and molar rotation of optically active substances.

CO4: Analyze and interpret the data collected by the methods discussed in the course.

Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

PRACTICALS

Spectrophotometry/ Colorimetry

1. To determine the strength of unknown solution of $CuSO_4.5H_2O$/$K_2Cr_2O_7$/$KMnO_4$ spectrophotometry/ colorimetrically and verify Lambert Beer's law.
2. Study the Cu^{2+} - EDTA complex by Job's method.
3. To find composition of Fe^{3+} ion thiocyanate (CNS) complex by Job's method.
4. Study the Cu^{2+}- EDTA complex by titration method.
5. Titration of Fe(II) with $KMnO_4$ by spectrophotometric method.
6. To determine the concentration of Ni (II) ions using EDTA by spectrophotometric method.

7. To determine the concentration of Cu (II) ion using EDTA by spectrophotometric method.
8. Titration of a solution of NaOH against HCl spectrophotometrically.
9. Titration of solution of Mohr's salt against EDTA solution spectrophotometrically.
10. To determine the dissociation constant of phenolphthalein.

Polarimetry

11. To find the specific rotation and molar rotation of optically active substances.
12. To compare the strength of HCl and H_2SO_4 acids.
13. To find the percentage of d-sugar and d-tartaric acid in the given solution.
14. To study the influence of solvent on the optical rotation of a solute. Also find specific and molar rotation.
15. To study influence of added impurity on the optical rotation of a solute.

Note: Subject to the availability of chemicals experiments can be substituted by alternate experiment.

Books Recommended:

1. Advanced Physical Chemistry Experiments, Gurtu-Gurtu.
2. Senior Practical Physical Chemistry, B.D. Khosla V.C Garg & Adarsh Gulati.
3. Practical Physical Chemistry, B.Viswanathan & P.S Raghavan.
4. Practical Physical Chemistry, A.M. James and F. E. Prichard, Longman.
5. Practical Physical Chemistry, Alexander, and Findley.
6. Advanced Practical Chemistry, Jagdamba Singh, R.K.P Singh, Jaya Singh.
7. Advanced Practical Chemistry, R. Mukhopadhyay and P. Chatterjee.
8. University Practical Chemistry, P.C. Kamboj.
9. Advance Practical Physical Chemistry, J. B. Yadav.
10. Textbook of Chemistry Practical, Bidhan Chandra Ray and Satyanarayan Das.

SEMESTER-III

MSCHE 301: Reaction Mechanisms of Transition Metal Complexes

Maximum Marks: 100		L T P 5 0 0
Semester Examination: 70		Lectures: 60
Internal Assessment: 30	Time: 3hrs	Pass marks: 35%

COURSE OUTCOMES

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

CO1: Interpret the mechanism of substitution in octahedral and square planar complexes.

CO2: Analyse the factors and predict the rates of substitution in octahedral and square planar complexes.

CO3: Comprehend the mechanisms of electron transfer reactions.

CO4: Identify and interpret mechanisms of oxidative addition, reductive elimination, insertion and migration reactions.

CO5: Analyze the factors affecting the stability of complexes and predict stability of complexes.

CO6: Apply various methods to determine the stoichiometry and stability of complexes.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions from each unit I, II and unit III is compulsory.

Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

Unit I

Reaction Mechanisms of Transition Metal Complexes:

Reactions of Octahedral Complexes**:** Ligand replacement reactions, substitution reactions in octahedral complexes, inert and labile complexes, mechanisms of substitution reactions (dissociative, associative, interchange), acid hydrolysis and base hydrolysis reactions, water exchange rates, formation of complexes from aqueous solutions, anation reactions of metal complexes, Reactions of Square Planar Complexes: Substitution reactions, mechanism of ligand displacement reactions, the *trans*-effect, theories of *trans*-effect, *cis*-effect.

Electron Transfer Reactions:

Electron transfer theory, mechanisms of electron transfer: inner sphere and outer sphere mechanisms, ligand bridged reactions, iron (II)-iron (III) exchange, two electron transfer reactions: complimentary and non-complimentary reactions, replacement through redox mechanism.

Unit II

Oxidative Addition and Migration Reactions:

General comments, the acid base behaviour of metal atom in complexes, Lewis acidity of complexes, oxidative addition: addition reactions of specific molecules (hydrogen addition, HX additions, addition of X_2, addition of organic halides, addition reactions of Si-H bonds), reductive elimination reactions, cleavage of C-H bonds, alkane activation, cyclometallation reactions, insertion reactions, insertion of CO, insertion of alkenes and C-C unsaturated compounds,

Metal-Ligand Equilibria in Solution:

Introduction, stepwise and overall formation constants, thermodynamic and kinetic stability, Factors affecting stability constants associated with metal and ligands, origin of statistical, electrostatic and chelate effect.

Determination of stability constants by following methods:

1. Slope ratio method
2. Job's method of continuous variation
3. Mole ratio method
4. Bjerrum's potentiometric method
5. Polarographic method of Deford and Hume
6. Ion-exchange method

Books Recommended:

1. *Advanced Inorganic Chemistry,* Cotton and Wilkinson, John Wiley (5th edition and
2. *Inorganic Chemistry,* K.P.Purcell and J.V. Kotz, W.B. Saunders Co. London (1977).
3. *Inorganic Reactions Mechanism, An Introduction* by Edwards W.A. Benzamin, Inc.
4. *Inorganic Chemistry,* Miessler and Tarr 3rd edition, Pearson Education.
5. *Inorganic Chemistry,* Shriver and Atkins, Oxford University Press. (4th edition).
6. *Inorganic Chemistry*, Huheey III and IV editions, Pearson Education Asia.
7. *Elementary Coordination Chemistry,* Jones and Jones.
8. *Polarography of Metal Complexes,* D. R. Crow.
9. *Instrumental Methods of Analysis,* D.A. Skoog.
10. *Concepts of Inorganic Photochemistry,* A. W. Adamson and P. D. Fleischauer, Wiley.
11. *Inorganic Chemistry: A Unified Approach*, W.W. Porterfield. (6th edition).

MSCHE 302: PHOTOCHEMISTRY AND PERICYCLIC REACTIONS

Maximum Marks: 100		L T P 5 0 0
Semester Examination: 70		Lectures: 60
Internal Assessment: 30	Time: 3hrs	Pass marks: 35%

COURSE OUTCOMES

On completion of the course students will be able to:

CO1: Construct a Jablonski diagram and explain the various photophysical processes.

CO2: Identify the product of the photochemical reaction under the given conditions.

CO3: Illustrate the mechanism and identify the stereochemical differences of photochemical reactions.

CO4: Analyse the photochemistry of alkenes and carbonyl compounds to predict the products of various photochemical reactions.

CO5: Distinguish between the type of rearrangement reactions and to make up the mechanism of the rearrangement reactions.

CO6: Apply the FMO and PMO approach of pericyclic reactions to predict the pathway of reaction.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory. Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT -I

Photochemical Excitations of the molecules. Energy of the molecule, Photochemical Energy, Electronic transitions– types of electronic Excitations and molecular orbital view of excitation, Spin multiplicity–nomenclature of excited states.

The fate of the excited molecules: Photophysical Processes- Jablonski diagram, Intersystem crossing, Energy transfer, Laws of Photochemistry, Quantum efficiency, sensitization and Quenching.

Photochemistry of Alkenes, Dienes, and aromatic compounds, Cis-trans isomerisation of alkenes, Dimerization of alkenes, Photochemistry of conjugated dienes.

Photochemistry of Carbonyl Compounds: α-cleavage or Norrish Type-I process, β- cleavage reaction or Norrish Type-II process, Intramolecular Hydrogen abstraction (γ- Hydrogen abstraction, δ-Hydrogen abstraction), Formation of Photo enols or Photoenolization, Photocycloaddition reaction (Peterno-Buchi Reaction), [2+2] Cycloaddition reaction of enones with alkenes.

UNIT-II

Photoisomerisation of benzene and substituted benzene, Photoaddition of alkenes to aromatic benzenoid compounds, Addition of oxygen, Aromatic photosubstitution, Photochemistry of Diazo compounds, Photochemistry of Azides.

Photorearrangements of Cyclopentanone, Cyclohexanone rearrangements, Rearrangements of Dienones, Photorearrangments of β, γ-unsaturated ketones, Aza-di-π- methane rearrangements, Di-π-methane (DPM) rearrangements, Rearrangements in aromatic compounds, Photo-Fries rearrangements.

The Frontier Molecular Orbital Approach and Perturbational Molecular Approach

Cycloadditions: Cheletropic reactions, 1,3-Dipolar cycloadditions.

Sigmatropic reactions: Claisen and Cope rearrangements, [2,3]-sigmatropic rearrangements and higher order rearrangements, Ene reaction. Peripatetic cyclopropane bridge, Fluxional molecules-degenerate Cope rearrangements.

Pericyclic Reactions Involving Ionic Transition States: Cycloaddition reactions, Electrocyclic reactions, Sigmatropic reactions, Peripatetic cyclopropane bridge, Cheletropic reactions, 1,3 Dipolar cycloaddition, Group transfers and Group eliminations.

Books Recommended:

1. *Fundamentals of Photochemistry,* K.K. Rohatgi Mukherji Reprint, Revised edition, New Age International (P) Ltd., Publishers New India.1997.
2. *Modern Molecular Photochemistry*, N.J. Turro, the Benjamin/Cummings Co., Inc. California, USA, 1978.
3. *Molecular reactions and photochemistry*, Charles H. Depuy and orville L.
4. Chapman, Prentice Hall of India Pvt. Ltd. New Delhi, India, 1972.
5. *Photochemistry of Excited states,* J.D. Coyle.
6. *Photochemistry and Pericyclic reactions*, Jagdamba Singh and Jaya Singh, New Age International Pvt. Limited, New Delhi.
7. Pericyclic *Reactions: A Textbook: Reactions, Applications and Theory,* R. Hoffmann and S. Sankararaman, Wiley India, 2015.

MSCHE 303: Advanced Physical Chemistry-I

Maximum Marks: 100		L T P 5 0 0
Semester Examination: 70		Lectures: 60
Internal Assessment: 30	Time: 3hrs	Pass marks: 35%

COURSE OUTCOMES

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

CO1: Illustrate the simple quantum mechanical models such as simple harmonic oscillator, particle in a one- and three-dimensional box, quantum mechanical tunneling, rigid rotor, Hydrogen atom etc.

CO2: Explain the quantum mechanical aspect of angular momentum and spin, approximations based on variation method and time independent perturbation theory.

CO3: List the applications of harmonic oscillator, rigid rotor, one-electron, and many electron atoms, and homo-and hetero-nuclear diatomic molecules.

CO4: Discuss the different theories of reaction rates and factors affecting reaction rates. Explain complex, gas phase, slow, fast, and oscillatory reactions.

CO5: Classify the different types of catalysis and their mechanisms.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Basics of quantum chemistry: Introduction of quantum chemistry, operators, postulates of quantum chemistry, eigen value and eigen function, normalization and orthogonality, Schrodinger wave equation using operators.

Applications of quantum chemistry to simple systems:

Translational motion: Particle in one dimensional box, particle in three-dimensional box rectangular and cubical box.

Vibrational motion: Harmonic oscillator, the quantum mechanical derivation for a harmonic oscillator model of a diatomic molecule, physical interpretation of ψ and ψ^2.

Rotational motion: Rigid rotator, derivation of energy and wave function of rigid rotator, rotation in one plane, rotation in space.

Application of quantum mechanics to Hydrogen and Hydrogen like particles: Hydrogen like particles, Schrodinger wave equation for Hydrogen-like particles, separation of variables, radial wave functions and angular wave functions.

Approximate methods: Variation principle, linear and non-linear variation theory, Perturbation theory, application of variation and perturbation theory to He atom.

Theory of angular momentum: Angular momentum, quantum mechanical operator for angular momentum, ladder operator, eigen function and eigen values of angular momentum using ladder operator, orbital and spin motion, spin angular momentum.

Molecular orbital theory (MOT): LCAO approximation, Huckel MOT of conjugated systems, Huckel rule of aromaticity, applications of Huckel MOT to ethylene, butadiene, charge density calculation, bond order, free valency, elementary idea of extended Huckel theory.

Unit -II

Chemical Kinetics

Recapitulation of Basic Concepts of Kinetics: Introduction, factors influencing on reaction rates, influence of temperature on reaction rates, order and molecularity of reaction, methods of determination of order of reaction.

Theories of reaction rates: Collision theory for bimolecular reaction, Transition state theory or the theory of absolute reaction rates (Eyring equation), thermodynamic formulation of reaction rates,

Elementary Gas-phase Reactions: Lindemann-Christiansen hypothesis. Hinshelwood's treatment. Rice-Ramsperger-Kassel (RRK) treatment. Slater's treatment. Rice-Ramsperger-Kassel Marcus (RRKM) treatments of unimolecular gas phase reactions.
Composite/Complex Reactions: Parallel reactions, reversible reactions, consecutive reactions.
Reaction in Flow Systems: Determination of fast reactions by NMR method, relaxation method, temperature jump method, pressure jump method, flow and stopped flow method.
Reactions in solution: Primary and secondary salt effects.
Oscillatory Chemical Reactions: Belousov-Zhabotinsky reactions. Classification of Oscillatory Reactions, Lotka-Voltera model.
Catalysis: Introduction, characteristics of catalytic reactions, types of catalysis: heterogeneous catalysis, homogeneous catalysis, organocatalysis, photocatalysis, autocatalysis, inhibitors and promoters, acid base catalysis, enzyme catalysis, Michaelis Menten equation, effect of temperature and pH on enzyme catalysis.

Books Recommended:

1. Elements of Physical Chemistry, Peter Atkins, Julio de Paula, Oxford University Press.
2. Chemical Kinetics, Keith J. Laidler, Prentice Hall.
3. Atkins Physical Chemistry, P.W. Atkins, C.A. Trapp, M.P. Cady, C. Giunta, Oxford Chemistry Press.
4. Principles of Physical Chemistry, B.R. Puri, L.R. Sharma & M.S. Pathania, Vishal Publishing Co.
5. Kinetics and mechanism, A. A. Frost & R.G Pearson, John-Wiley, & Sons Inc., N. York.
6. Chemical kinetics methods, C. Kalidas, New Age International Pvt. Ltd. Publishers.
7. Principles of Polymerization, George Odian.
8. Principles of Polymer Chemistry, Paul J. Flory.
9. Textbook of Physical Chemistry, Glasstone.
10. Text book of Physical Chemistry, G.M.Barrow

MSCHE 304: Chemistry Practicals

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

On completion of the course, students will be able to

CO1: Perform conductometric and pH metric titrations.

CO2: Apply chromatographic techniques including paper, thin layer, and column chromatography for carrying out separation of substances.

CO3: Use computers-based tools for presenting data, literature search, drawing structures, and optimisation of parameters.

CO4: Develop skills in observation, scientific thinking and problem solving.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:

Experiment I: 35 marks

Experiment II: 35 marks

Viva-Voce: 20 marks

Practical Record Book: 10 marks

Inorganic Chemistry Practicals

Conductometry

1. Determination of number of ions in $[Co(NH_3)_6]Cl_3$, $[Hg(NH_3)_2Cl]$.
2. Titrations of mixture of acids.
3. Precipitation titrations.

pH-metric titrations

1. Acid-base titrations.
2. Mixture of acid with a base.

Chromatographic separations

1. Separation of ions by Paper chromatography.

2. Separation of ions by Column chromatography.

Computers based Practicals.

1. Use of MS Office for evaluation and presentation of data (plotting of graphs, finding fit, correlation coefficient)
2. Drawing structures of molecules and optimisation of parameters using free chemistry softwares like Chemsketch
3. Molecular modelling and optimisation of parameters using softwares like Argus Lab (www.planaria-software.com), WebLab Viewer, Hyperchem, TINKER 6.0 (dasher.wustl.edu/ffe) etc.
4. Literature search using search engines, databases and website like Google scholar, ScienceDirect, Scinapse, acs

Books Recommended:

1. *Advanced Practical Inorganic Chemistry,* D.M. Adams and J.B. Raynor, John- Wiley & Sons, Ltd.
2. *Experimental Inorganic Chemistry*, W.G. PALMER, Cambridge at University Press.
3. *Advanced University Practical Chemistry,* P.C. Kamboj, Vishal Publishing Co.
4. *Advanced Practical Inorganic Chemistry,* Gurdeep Raj, Goel Publishing House.
5. *Advanced Physical Chemistry Experiments*, Gurtu-Gurtu.
6. *Advance Practical Physical Chemistry,* J. B.Yadav.
7. *Practical Physical Chemistry,* B.Viswanathan & P.S Raghava.

MSCHE 311: INORGANIC SPECTROSCOPY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

On completion of the course, the student should be able to

CO1: Explain the working principle of various spectroscopy techniques listed in course.
CO2: Explain and relate formalisms to predict spectroscopic properties.
CO3: Illustrate the applications of studied spectroscopic techniques in structural analysis.
CO4: Analyze the spectroscopic data collected by the methods discussed in the course and predict structure of inorganic compounds.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory. Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

IR, Raman and Microwave Spectroscopy:
Selection rules regarding IR and Raman scattering spectroscopy, fundamentals, overtones and combinations in vibrational spectroscopy, mutual exclusion principle, symmetry symbols for normal modes of vibration, IR and Raman activity of their fundamentals and nature of vibrations in terms of change in internal coordinates in simple molecules like trans N_2F_2, SF_6.

Applications of Raman and IR selection rules to the determination of Inorganic structure with special emphasis on:

i) Metal carbonyls
ii) NSF_3
iii) Geometrical isomerism-differentiation between Cis and trans. $[Co(bipy)_2Cl_2]Cl$
iv) Structures of CO_2, N_2O, H_2O, chlorocomplexes of mercury, cadmium and zinc and some octahedral complexes ML_6 (SiF_6^{2-}, PF_5^-, SF_6)
v) Changes in the spectra of donor molecules upon coordination with special emphasis on N, N-dimethylacetamide and DMSO with Fe^{3+}, Cr^{3+}, Zu^{2+}, Pd^{2+} and Pt^{2+}ions.

I.R spectroscopy and modes of coordination of SO_4^{2-}, N_2, O_2, NO, CO_3^{2-}, NO_3^-.

Microwave Spectroscopy**:** Theory, selection rules and intensities of spectral lines, applications of microwave spectroscopy.

Photo Electron Spectroscopy

Introduction, excitation & ejection of electrons, electronic energy levels in atoms and molecules, Core level photoelectron spectroscopy, symmetry & molecular orbitals, valence electron photo electron spectroscopy, valence excitation spectroscopy. Dissociation, Predissociation, change of shape on excitation.

UNIT-II

Electron Paramagnetic Resonance Spectroscopy

Introduction, similarities between EPR and NMR, behaviour of free electron in an external magnetic field, basic principle of EPR, the hydrogen atom, presentation of the spectrum, hyperfine splitting in isotropic systems involving more than one nucleus, contributions to hyperfine coupling constant in isotropic systems. Anisotropy in the g-value, EPR of triplet states, nuclear quadrupole interaction, line widths in EPR, applications of EPR.

Nuclear Quadruple Resonance

Nuclear electric quadruple moment, electric field gradient, energy levels, effect of magnetic field on spectra, factors affecting the resonance signal, relationship between the electric field gradient and molecular structure.

Applications: Interpretation of NQR data, structural information of the following: Application ($PFCI_4.PCI_5$), $(NH_4)_2TeCl_6$, group 14 tetra halides, R_3MX_2 (M=As, Sb, Bi), Cis & Trans$[Co(en)_2Cl_2]Cl$, Polyhalide ion, BrCN, HIO_3

Mössbauer Spectroscopy

Introduction, principle, conditions for mössbauer spectroscopy, parameters from mössbauer spectra, isomer shift, electric quadrupole interactions, magnetic interactions mb experiment, application of MB spectroscopy in structural determination of the following:

i) High spin Fe (II) and Fe (III) halides: FeF_2, $FeCl_2.2H_2O$, FeF_3, $FeCl_3.6H_2O$.

ii) Low spin Fe (II) and Fe (III) Complexes: ferrocyanides, ferricyanides, prussian blue.

iii) Iron carbonyls: $Fe(CO)_5$, $Fe_2(CO)_9$ and $Fe_3(CO)_{12}$.

iv) Inorganic Sn (II) and Sn (IV) halides.

Books Recommended:

1. *Physical methods for Chemists,* R.S. Drago.
2. *Structure Methods in Inorganic Chemistry*, E.A.V Ebsworth and W.H Renkin.
3. *Molecular Spectroscopy,* C.M. Banwell.
4. *Spectroscopy*, S. Walker and H. Straugh Vol.I,
5. *Infrared Spectra of Inorganic and co-ordination Compounds*, K. Nakamoto
6. *Electron Spin Resonance*, E. Wertz and J.R. Bolton.
7. *Mossbauer Spectroscopy*, N.N. Greenwood and T.C. Tibb
8. *Chemical application of Spectroscopy in Inorganic Chemistry,* C.N.R. Rao.

MSCHE 312: INORGANIC CHEMISTRY PRACTICALS-II

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Lectures: 60
Time: 6 hours

COURSE OUTCOMES

On completion of the course, the student will be able to

CO1: Prepare various coordination compounds.
CO2: Demonstrate comprehensive understanding of the stereochemistry of synthesized compounds.
CO3: Record and analyse the properties viz. UV-Vis and IR spectra of synthesised compounds.
CO4: Exhibit skills to design and carry out experiments in order to analyse and find out the composition of alloys.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:
Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

A. Preparation of following compounds and study of their important properties viz.
UV-Vis and IR spectra.

1. Preparation of $(NH_3)_2HgCl_2$ and estimation of Hg.
2. Mercuration of phenol and separation of the compound into ortho and para isomers.
3. Preparation of vanadylacetylacetonate $VO(acac)_2$ and its pyridine complex, and estimation of V(IV).
4. Preparation of cis and trans potassium dioxalatodiaquochromate(III), estimation of Chromium (ref. Marr and Rockett, 1972, page 386).
5. Preparation of $[Ni(NH_3)_6]Cl_2$ its characterization and estimation of Ni(II)

6. Preparation of Nitrosylbis(diethyldithiocarbamate) iron (I).
7. Preparation of Chloropentaammminecobalt(III) chloride, $[Co(NH_3)_5Cl]Cl_2$.
8. Preparation of cis and trans bis(ethylenediaminecobalt(II) chloride.
9. Preparation of Dipyridiniumhexachloroplumbate.
10. Preparation of bis(acetylacetonato)copper(II)
11. Demonstration of Jahn Teller effect by solution spectral studies. (ref. Bull. Chem. Soc. Japan, 1965, 29, 852).

B. Synthesis and characterization of the Ni (II) complex of a Schiff-base ligand derived from salicylaldehyde and ethylenediamine.

C. Analysis of Alloys (Brass, bronze, solder).

Books Recommended

1. *Practical Inorganic Chemistry,* G. Marr, B. W. Rockett, (1972).
2. *Inorganic Chemistry,* I. Grenthe, E. Nordin, 18 (1979) 1869–74.
3. *Inorg. Synth.*, J.C. Bailar, M. Eldon, 1 (1939) 35–38.
4. *Advanced University Practical Chemistry,* P.C. Kamboj, Vishal Publishing Co.
5. *Advanced Practical Inorganic Chemistry,* Gurdeep Raj, Goel Publishing House.

MSCHE 321: HETEROCYCLIC CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

On completion of the course, the student should be able to

CO1: Name heterocycles using various methods of nomenclature.

CO2: Understand the criteria of aromaticity in heterocycles and the outcomes of steric and stereo electronic effects in non-aromatic heterocycles.

CO3: Gain understanding of various methods for ring synthesis and application of those methods for the preparation of specific groups of heterocyclic systems.

CO4: List the synthetic methods and reactions of important three, four, five and six heterocycles.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT I

Nomenclature of Heterocycles: Replacement and systematic nomenclature (Hantzsch- widman System) for monocyclic fused and bridged Heterocycles.

Aromatic Heterocycles: General chemical behaviour of aromatic heterocycles classification (structural type) criteria of aromaticity (bond length ring current and chemical shift in H NMR-

Spectra empirical resonance energy delocalization energy and Dewar resonance energy Diamagnetic susceptibility exaltations).

Non-aromatic Heterocycles: Strain-bond angle and torsional strains and their consequences in small ring heterocycles. Conformation of six-membered heterocycles with reference to molecular Geometry, barrier to ring inversion, pyramidal inversion and 1, 3-diaxial interaction. Stereoelectronic effects- anomeric and related effects. Attractive interactions-hydrogen bonding and intermolecular nucleophilic-electrophilic interactions.

Three membered rings with one heteroatom: Oxirane, Aziridine, Thirane: Introduction, synthetic methods, Direct insertion of heteroatom into carbon-carbon-double bond, methylene insertion reaction, cyclisation method, condensation reaction, Nucleophillic and Electrophillic ring opening. Reaction involving extrusion of the heteroatoms.

UNIT II

Four membered Heterocyclics with one Heteroatom: Oxetane, Oxetene, thitenes, thitanes, Azitidines: Introduction, Synthetic method, Cyclisation reaction, Direct combination method, Reaction electrophilic, nucleophilic ring opening and General chemical reactions.

Five membered Heterocyclics with two heteroatoms: Pyrazole and Imidazoles: Introduction, Physical properties, Structure, Synthetic method, Electrophillic and Nucleophillic reactions. Isoxazole and Oxazole: Introduction, Physical and chemical properties of isoxazole and oxazoles and their derivatives. Isothiazole and Thiazoles: Physical and chemical properties, synthetic reactions.

Six membered Heterocyclic with two heteroatoms: Introduction: Pyridazine, Pyrimidine, Pryazine. Synthetic approaches. Chemical reactions; Electrophillic substitution, Nucleophilic substitution, Side chain reactivity. Oxazines: Classification, nomenclature structure, Synthetic approaches, and chemical reactions.

Books Recommended:

1. An *Introduction to the Chemistry of Heterocyclic Compounds*, Acheson, R.M. 3rd
2. Edition, John Wiley, 1976.
3. *Handbook of Heterocyclics,* A. R. Katrizky.
4. *Principles of Modern Heterocyclic Chemistry,* Lee A. Paquette.
5. *Molecular Rearrangement,* P-de-Mayo. Vol.1.
6. *Heterocyclic Chemistry,* Gupta, R.R.; Kumar, M.; Gupta, V Vol. 1-3, Springer Verlag, 1998.
7. *Heterocyclic Chemistry*, Joule, J.A.; Mills, K.; Smith, G. F. 3rd edition, Chapman and Hall, 1998.

8. *Comprehensive Heterocyclic Chemistry*, Katrizky, A.R.; Rees, C.W. 2nd Edition, Pergamon Press, 1997.

MSCHE 322: Organic Chemistry Practicals-II

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

After the completion of this course student will be able to
CO1: Prepare organic compounds via multi step synthetic sequences.
CO2: Know the various methods employed for synthesis of organic compounds.
CO3: Monitor the progress of a reaction.
CO4: Learn the characterization of the synthesized compounds.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:
Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

Multistep Synthesis

1. **Beckmann Rearrangement**

   i. Benzophenone- Benzophenone Oxime- Benzanilide.
   ii. Acetophenone- Acetophenone Oxime- Acetanilide.

2. **Benzillic acid Rearrangement**

   i. Benzoin-Benzil-Benzillic acid.
   ii. Benzoin-Benzil-Benzilmonohydrazone.

3. **Fischer Indole Synthesis**

i. 1, 2, 3, 4 tetrahydrocarbazole.
ii. 2-Phenyl Indole from Phenyl hydrazone.

4. p-Bromo/ Nitro acetanilide from aniline

i. To prepare Acetanilide from Aniline (Acetylation).
ii. To prepare p-bromoacetanilide from Acetanilide (Bromination).
iii. To prepare p-nitroacetanilide from Acetanilide (Nitration).

5. Photochemical Reaction

i. Benzophenone to Benzpinacol.

Students are supposed to know the IR and NMR Spectra of prepared compounds and how to monitor the progress of a reaction.

Note: *Subject to the availability of chemicals experiments can be substituted by alternate experiment.*

Books Recommended:

1. *Practical Organic Chemistry*, Mann, F.G & Saunders, B.C., Pearson Education.
2. *Practical Organic Chemistry*, Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G. & Tatchell,
3. A.R. 5th Ed. Pearson.
4. *Quantitative Organic Analysis,* Arthur I. Vogel, 2nd Ed. Pearson.

MSCHE: 331 Chemical Thermodynamics

Maximum Marks: 100		L T P 5 0 0
Semester Examination: 70		Lectures: 60
Internal Assessment: 30	Time: 3hrs	Pass marks: 35%

COURSE OUTCOMES

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

CO1: Recall the basic definitions of chemical thermodynamics. Apply the first, second and third law of thermodynamics for different systems. Define the concept of thermodynamic probability.

CO2: Explain about the statistics of photon and electron gases, thermionic emission, partition function.

CO3: Illustrate the various kinds of Fluctuation. List the salient features of Non equilibrium or Irreversible Thermodynamics.

CO4: Compare the different types of thermo electric phenomena-The Seebeck effect, Peltier effect and Thomson effect.

CO5: Apply the principles of statistical mechanics to selected problems.

INSTRUCTIONS FOR THE PAPER-SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory. Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Basics of Chemical Thermodynamics:
Thermodynamic Properties, State and path properties, first and second law of thermodynamics, Maxwell relations, thermodynamic equation of state, Joule Thomson effect, Nernst heat theorem, thermodynamic entropy, third law thermodynamics, Identification of statistical and thermodynamic entropy, determination of absolute entropies of solids, liquids, and gases.
Non ideal system: Excess thermodynamic functions, determinations of partial molar properties, fugacity and activity, fugacity of gases and experimental determination of fugacity, fugacity of mixture of gases, determination of activity and activity coefficients of non-electrolytes.
Thermodynamics of living systems: General thermodynamic consideration of living systems. simultaneous or coupled reactions, coupled reactions and metabolism, free energy utilisation in metabolism, terminal oxidation chain, overall metabolic plan.
Non equilibrium or Irreversible Thermodynamics
Thermodynamics of irreversible processes, silent features of non-equilibrium thermodynamics, stationary state, simple example of irreversible processes. general theory of near equilibrium processes, entropy production from heat flow, matter flow and current flow, generalized equation for entropy production, The phenomenological relations, Onsager reciprocal relation (without derivation), applications of Onsager theory to chemical reactions : coupled and uncoupled reactions and relaxation processes, application of irreversible thermodynamics to diffusion, thermal diffusion, thermo osmosis and thermo molecular pressure difference, thermoelectric phenomena, the Seebeck effect. Peltier effect, Thomson effect.

UNIT-II

Statistical Thermodynamics: Microstates and macrostates, concept of distribution, thermodynamic probability, and most probable distribution. Ensembles, Lagrange's undetermined multipliers, Sterling's approximation, types of statistics, derivation of distribution laws for Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics, molecular partition function and its importance, translational, rotational, vibrational, electronic, and nuclear partition functions, expression for internal energy, entropy, Helmholtz function, Gibb's free energy, pressure, work and heat in terms of partition function.
Quantum Statistics: Statistics of photon and electron gases, velocity, speed, and energy distribution functions. Principle of equipartition of energy. barometric equation, theory of paramagnetism, statistics of photon and electron gases, Thermionic emission.

Applications to Ideal gases: The molecular partition function and its factorization evaluation of translational, rotational, and vibrational partition function for monoatomic, diatomic and polyatomic gases, the electronic and nuclear partition functions, Ortho and para hydrogen, statistical weights of ortho and para states, symmetry number, Einstein theory of heat capacity, Limitation of Einstein theory, Lennard-Jones potentials energy equation compressed gases.

Solid State: Classical treatment of specific heat of solids. Einstein and Debye theories of specific heat, Debye T^3 law, entropy of solids, equation of state of solids, order and disorder and the melting point, Fluctuations Means distribution, mean square deviation, fluctuation in energy in a canonical ensemble, density fluctuation in a gas, Theory of Brownian motion, and Brownian motion of galvanometer.

Books Recommended:

1. C. Kalidas and M.V. Sangaranarayanan : Non – Equilibrium Thermodynamics .
2. Prigogine: Non – Equilibrium Thermodynamics.
3. Advanced Physical Chemistry, J.N. Gurtu and A. Gurtu, Pragati Prakashan.
4. M.C. Gupta: Statistical Thermodynamics
5. Terrell L Hill: An introduction to Statistical Thermodynamics.
6. Molecular Thermodynamics, Richarson E. Dickerson, W.A. Benjamin.
7. Thermodynamics for Chemists, Samuel Glasstone, Affiliated East-West Press Pvt. Ltd.
8. Principles of Physical Chemistry, B.R. Puri, L.R. Sharma & M.S. Pathania, Vishal Publishing Co.

MSCHE 332: Physical Chemistry Practicals-II

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

On completion of the course students will be able to:

CO1: Determine association factor, dissociation factor, enthalpy of vaporisation, integral heat of dilution of acid ie. at different concentrations, find heat of precipitation, heat of hydration and heat of transition of different salts.
CO2: Learn how to perform practical of kinetics to calculate order of reaction, activation energy, also learn about clock reaction.
CO3: Able to know about boiling point of two-component system. Relationship between solubility of two liquids of completely and partially mixing in each other.
CO4: Application of triple systems phase base component. Set the coefficient of distribution of acetic acid between chloroform and water.

Practicals

1. To determine association factor of oxalic acid from solubility measurements.
2. To determine the heat of neutralisation of acetic acid by sodium hydroxide and from it also calculate the heat of ionisation of acetic acid.
3. To determine integral heat of dilution of sulphuric acid starting with 10 M acid and going down by 9 M,8M,7M,6M, and 5M.
4. To determine the order of saponification of ethyl acetate with NaOH.
5. To study the kinetics of reaction between potassium bromate and potassium iodide in acidic medium at room temperature.
6. To study the kinetics of reaction between potassium bromate and potassium iodide in acidic medium at three temperatures and hence to find out the activation energy of the reaction.
7. To study the reaction between H_2O_2 and HI by clock method at three temperatures, and hence to find out the activation energy of the reaction.
8. To study manganese catalysed bromate-malonic acid reaction.
9. To determine the CST and CSC for phenol/water system and study the effect of impurity on miscibility temperature of phenol water system.

10. To find the eutectic point for two component system (naphthalene/benzoic acid) or (benzoic acid/ cinnamic acid)
11. To study the limit of homogeneity of three components: ($C_6H_5CH_3$, CH_3COOH, and H_2O) or ($CHCl_3$, CH_3COOH, and H_2O) system.

Books Recommended:

1. Advanced Physical Chemistry Experiments, Gurtu-Gurtu:.
2. Senior Practical Physical Chemistry, B.D.Khosla V.C Garg & Adarsh Gulati:
3. Practical Physical Chemistry, B.Viswanathan & P.S Raghavan :.
4. Practical Physical Chemistry, A.M. James and F. E. Prichard, Longman
5. Practical Physical Chemistry, Alexander, and Findley.
6. Advanced Practical Chemistry, Jagdamba Singh, R.K.P Singh, Jaya Singh.
7. Advanced Practical Chemistry, R.Mukhopadhyay and P. Chatterjee.
8. University Practical Chemistry, P.C. Kamboj.
9. Advance Practical Physical Chemistry, J. B.Yadav.
10. Textbook of Chemistry Practical, Bidhan Chandra Ray and Satyanarayan Das:

SEMESTER-IV

MSCHE 401: CHEMISTRY OF ORGANOMETALLIC COMPOUNDS

Maximum Marks: 100		L T P 5 0 0
Semester Examination: 70		Lectures: 60
Internal Assessment: 30	Time: 3hrs	Pass marks: 35%

COURSE OUTCOMES

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

CO1: Relate the concepts of organometallic chemistry in various organomatellic reactions.

CO2: Explain the basic organometallic concepts and understand the synthetic and mechanistic aspects.

CO3: Illustrate and relate organometallic concepts to synthesis, mechanisms and the functions of various organometallic reagents or catalysts.

CO4: Correlate the industrially important catalytic processes through the application of organometallic principles.

CO5: Evaluate the application of organometallic concept to some important organometallic compounds, homogeneous catalysis process and metal carbonyls.

CO6: Propose a solution about structure and bonding issues to understand the stability and reactivity of metal carbonyls.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.

Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Organometallic Compounds:
Nomenclature of organometallic compounds, types of ligands and their classifications in organometallic compounds, EAN rule, electron count in some organometallic compounds, Energy polarity and reactivity of M-C bond, stability of main group organometallics: methods of preparation in perspective-organolithium compounds: structure and bonding & reaction, carbolithiatic organometallics of group 2 and 12 e.g. Mg and Zn, Cd and Hg: preparation and structure of organoaluminium compounds, technical applications of tris (alkyl) aluminium compounds,. compounds with transition metal single, double and triple bonds to carbon.
Synthesis, structure, and bonding aspects of some important organometallic compounds.

a) η^1alkyl, alkenyl, alkynyl and aryl ligands.
b) η^2alkene and alkyne complexes of transition metals.
c) η^4 Butadiene and cyclobutadiene complexes of transition metals.
d) η^5 cyclopentadiene complexes of transition metals (special emphasis to ferrocenes).
a) η^6 – ligands: benzene and its derivatives, multidecker sandwich compounds.

UNIT-II

Homogenous Catalysis by Transition Metal Complexes:
hydrogenation reactions, alkene isomerisation, hydrosilation and hydroboration reactions, alkene hydrocyanation, reactions of carbon monoxide and hydrogen: the water gas shift reaction, the FischerTropsch reaction; hydroformylation of unsaturated compounds, alcohol carbonylation, Zeigler Natta polymerization of ethene and propene, alkene dimerization and oligomerizations, reactions of conjugated dienes, reactions of alkynes, valence isomerisation of strained hydrocarbons, alkene and alkyne metathesis, oxidative carbonylations, alkene oxidations (Wacker process), alkane oxidations.

Transition Metal Carbonmonoxide Compounds:
preparation of metal carbonyls: mononuclear, binuclear, trinuclear, tetranuclear, and larger polynuclear carbonyls. Additional structural and bonding features: CO as pi acid ligand, fluxionality, semi bridging CO groups, side on bonding to CO, oxygen to metal bonds, vibrational spectra of metal carbonyls, detection of bridging CO groups, molecular symmetry from the number of bands, bond

angles and relative intensities, force constants, prediction and assignment of spectra, carbonylate anions, metal carbonyl hydrides, fluxional organometallic compounds.

Books Recommended:

1. *Advanced Inorganic Chemistry by Cotton and Wilkinson,* John Wiley and Sons, Inc.
2. (5^{th} and 6^{th} editions).
3. *Inorganic Chemistry,* Shriver, Atkins and Longford, Oxford University Press 1990.
4. *Inorganic Chemistry, J.E*. Huheey.
5. *Organometallic Chemistry,* R.C. Mehrotra.
6. *Organometallic compounds of transition metals*, R.H. Crabtree.
7. *Homogenous transition metal catalysis,* Christopher Masters.
8. C. Elschenbroich and A. Salzer, Organometallics: A Concise Introduction, 2_{nd} Ed., VCH 1992.
9. G. L. Miessler, D. A. Tarr, Inorganic Chemistry, 3_{rd} edition, Pearson Education

MSCHE 402: NAME REACTIONS AND REAGENTS IN ORGANIC SYNTHESIS

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

On completion of the course, the student should be able to

CO1: Get insights into reactions and reagents in organic synthesis.

CO2: Identify the various name reactions with examples.

CO3: Explain the utility of synthetic reagent for oxidation and reduction of various organic compounds.

CO4: Compare the action of various oxidising and reducing agents with respect to the chemoselectivity, regioselectivity and enantioselectivity.

CO5: Evaluate the organic reactions based on the influence of the functional group on substrate molecules, nature of reagent and the parametric conditions.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Reactivity, selectivity (stereoselectivity and chemoselectivity) and mechanistic approach of reduction reaction:

Catalytic Hydrogenation (Pt, Pd, Ru, Raney Ni, Tristriphenylphosphine rhodium chloride), Reduction with Hydride transfer reagents ($LiAlH_4$, $NaBH_4$, B_2H_6, Me_3SiH, di-isobutyl aluminium hydride). Reduction by dissolving metals: – Reduction by Sodium, Reduction with Zn, Clemmensen reduction, Birch Reduction. Baker's Yeast (enzymatic reduction), Catalytic reduction (Lindlar's catalyst, Rosenmund's reduction).

Reactivity and selectivity (stereoselectivity and chemoselectivity) and mechanistic approach of oxidation reactions:

Oxidation with ozone (O_3), Peracids, Lead tetraacetate $Pb(OAc)_4$, Periodic acid (HIO_4), Osmium tetraoxide (OsO_4), Potassium permanganate ($KMnO_4$), Nitric acid (HNO_3), Selenium oxide (SeO_2). Oxidation with DDQ, Chloranil and Oppenauer oxidation. Oxidation with Cr (VI) ($K_2Cr_2O_7$, Jone's reagent, Collin's reagent, PCC, PDC, Chromyl Chloride), Woodward and prevost hydroxylation, Reactivity and selectivity of oxidation.

UNIT-II

Some Special Reagents/Name reactions in Synthesis

Octacarbonyldicobalt, Pentacarbonyliron, Dicyclohexylcarbodiimide (DCC), Diazomethane, 1,3-Dithane Merrifield resin, Phase transfer catalyst and its applications, Crown ethers, Lithium diisopropylamide (LDA). Regioselective reagents of alkyl borane (9BBN, Sia_2BH, Ipc_2BH), Grubb's catalyst, Tebb's catalyst, Apple reaction and Nef reaction.

Organometallic Reagents

Methods of preparation and applications of Organonickel (Negishi reaction), Organotin, Organocuprate (Gillman's reagent), Organosilicon, Organochromium compounds (including Nozaki-HiyamaKishi reaction), Organopalladium (including Heck reaction, Stille coupling, Suzuki reaction, Sonogashira coupling).

Selective Rearrangments in Organic Synthesis

Mechanism and applications of the following rearrangements: Favorskii rearrangement, Wagner-Meerwein, Lossen, Curtius, Beckmann rearrangements.

Books Recommended:

1. *Advanced Organic Chemistry-Reaction, Mechanism and Structure,* Jerry March, John Wiley.
2. *Advanced Organic Chemistry,* F.A. Carey and R.J. Sundberg, Plenum.

3. *Modern Organic Reactions,* H.O. House, Benjamin.
4. *Organic Chemistry Reactions and Reagents*, O.P. Aggarwal, Goel Publishing House,
5. Meerut.
6. *Reactions, Rearrangements and Reagents,* S.N. Sanyal, BharatiBhawan.
7. *Applications of Redox and Reagents in Organic Synthesis,* Dr. Ratan Kumar Kar. New Central Book Agency, Delhi.
8. *Name Reactions in Organic Synthesis,* Dr. Arun R. Parikh, Dr. Hansa Parikh, Foundation Books, Delhi.
9. *Modern's Synthetic Reactions,* Carruthers.
10. *Reagents in organic synthesis,* Jagdambha Singh, L.D.S Yadav

MSCHE 403: Atmospheric Photochemistry

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

On completion of the course students will be able to:

CO1: Construct Jablonski diagram and explain the various photophysical processes. Discuss industrial applications of photo chemistry.

CO2:. Apply knowledge about photochemical and photo physical processes and the reactivity of excited states to explain applications in photochemical energy conversion and other selected issues.

CO3: Demonstrate the chemical and biochemical principles of fundamental environmental processes. Recognize different types of toxic substances and responses and analyse toxicological information. Apply basic chemical concepts to analyse chemical processes involved in different environments in air.

CO4: Describe causes and effects of environmental pollution by the energy industry.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

Photochemistry

Introduction, characteristics of electromagnetic radiation, difference between thermochemical and photochemical reactions, Lambert-Beer's law and its limitations, laws of photochemistry, Jablonski diagram, quantum yield, determination of quantum yield, examples of low and high quantum yields, photochemical reactions, photochemical rate law , energy transfer in photochemical reaction, photosensitization and quenching, Stern Volmer equation, rates of intramolecular photophysical processes and intramolecular energy transfer, photochemical degradation of excited states of Hg atoms, Hg sensitized photoreactions of simple alkanes and alkenes, luminescence, chemiluminescence, photosensitization, photo inhibitors, fluorescence and phosphorescence photo electrochemistry, hot atoms and its reactions, fluorescence and its measurement, excimer and exciplex formation.

Kinetics of Dynamic Chain Reactions: Hydrogen-bromine reaction. Hydrogen-chlorine reaction. Pyrolysis of acetaldehyde. Decomposition of ethane.

Industrial applications of Photochemistry: Technical applications, application of luminescence phenomena to optical bleaching of textiles and papers, non-radiative decay to ground state, applications of electron and energy transfer processes, photo fragmentations used in photochemical synthesis of detergent and insecticides.

UNIT-II

Structure of the atmosphere: Structure of the atmosphere in terms of temperature, characteristics and chemical composition, particles, ions and radicals in atmosphere, chemical and photochemical reactions in atmosphere, **Atmospheric photochemistry of following compounds** : Nitrate radicals, nitrous acid, nitric acid, ammonia, oxygen .

Ozone layer chemistry: The ozone layer in the stratosphere. ozone hole, chemistry of upper atmosphere.

Solar radiation: Solar spectral distribution outside the earth's atmosphere, absorption by N_2, O_2 O_3 and distribution of solar energy on earth.

Air Pollution: Air pollutants, CO_x, NO_x, SO_x, H_2S, hydrocarbons, organo sulphur, and organo nitrogen compounds as atmospheric pollutants, photochemical smog, adverse effects of smog, fluorine and other halogenated organic compounds, particulate matter, formation of organic and inorganic particulate matter.

Toxic chemicals in the environment, effects of atmospheric pollution, sinks of atmospheric gases, acid rain, adverse effects of acid rain, control of acid rain, aerosols and their effects, greenhouse effect, global warming.

Books Recommended:

1. Photochemistry, Gilbert & Cundel.
2. Photochemistry, Calvert & Pits.
3. Atmospheric Chemistry, Academic Press, New York, J. Heicklen.
4. Photochemistry, K.K. Rohtagi –Mukherjee
5. Environmental Pollution Control Engineering, New Age International (P) limited publisher, C.S. Rao.
6. Environmental Chemistry, A.K. De.
7. Environmental Chemistry, H Kaur.

MSCHE 404: CHEMISTRY PRACTICALS-II

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:
Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

COURSE OUTCOMES

On completion of this course students will be able to
CO1: Know the methods for calibration and sampling applied to quantitative analysis.
CO2: Measure the percentage purity of samples with functional groups such as hydroxyl, amine or carboxylic acids.
CO3: Record and analyze the results of quantitative analysis.
CO4: Determine the percentage purity of sugar by Fehling's method and Benedict's solution.
CO5: Critically evaluate data collected to determine the identity, purity, and percent yield of product.
CO6: : Perform the practicals of photochemistry mentioned in the course .Explain and calculate the concept of Quantum yield of the reaction.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:
Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

Quantitative Estimations

1. Hydroxyl group (Phenolic)

i. Determine percentage purity of given phenols by brominating reagent.

ii. To determine the percentage purity of given sample of *m*-cresol by using brominating reagent.

2. Amine group

i. Determine the amount of aniline per litre by substitution method.

ii. Determine the amount of *m*-toluidine in the given sample by brominating reagent.

iii. Find percentage purity of given sample of *m*-nitroaniline by brominating reagent.

3. Carbonyl group

i. To standardise the given glucose solution by Fehling's method.

ii. II. Determine the percentage purity of sugar by Fehling's method.

iii. To determine the amount of glucose in given sample by Benedict's Solution.

iv. To determine the amount of sucrose in a given sample by Benedict's method.

v. To hydrolyse the given sample of jaggery and determine the amount of glucose present in it by Benedict's Solution.

4. Acetous Perchloric Acid

i. To standardise acetous perchloric acid using primary standard potassium hydrogen phthalate.

ii. To determine percentage purity of sodium benzoate.

iii. To determine percentage purity of sodium salicylate.

iv. To determine percentage purity of given alkaloid (Ephedrine). V.

v. To find percentage purity of Brucine.

5. Intensity of the lamp/Quantum yield of the reaction

i. To draw calibration curve for various concentrations of FeSO4/1-10-phenanthroline complex and hence to find the coefficient of its molar absorptivity.

ii. To find out the intensity of the lamp (visible light) by ferrioxalate actinometer.

6. **Methylene blue sensitized photo oxidation of diphenylamine.**

i. To study the rate of formation of the product in the above photochemical reaction with increasing quanta of light absorbed and to find the quantum yield of this reaction.

Books Recommended:

1. Mann, F.G & Saunders, B.C., *Practical Organic Chemistry*, Pearson Education.
2. Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G. & Tatchell, A.R. *Practical Organic Chemistry* 5th Ed. Pearson.
3. Arthur I. Vogel *Quantitative Organic Analysis* 2nd Ed. Pearson.
4. Advance Practical Physical Chemistry, J. B.Yadav.
5. Textbook of Chemistry Practical, Bidhan Chandra Ray and Satyanarayan Das.

Note: *Subject to the availability of chemicals experiments can be substituted by alternate experiment*.

MSCHE 411: ADVANCED INORGANIC CHEMISTRY

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

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

CO1: Explain the synthesis methods, summarise structural patterns and predict the structure of clusters.

CO2: Explain various aspects of radioactivity, nuclear processes, and application of radioactive elements in isotopic and exchange reactions.

CO3: Interpret the role of metal ions in biological systems.

CO4: Summarise the principles of receptor design and the role of receptors in recognition, transformation, and transport.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Cluster Compounds:

Molecular structures of clusters, metal carbonyl clusters, stereochemical non-rigidity in clusters, electronic structures of clusters with π-acid ligands, isoelectronic and isolobal relationships, structural pattern and synthesis of High Nuclearity Carbonyl Clusters (HNCC's), Electron counting scheme for HNCC's, the capping rule, isoelectronic and isolobal relationship, hetero atoms in metal atom clusters: carbide and nitride containing clusters, HNCC's of Fe, Ru, Os, Co, Rh, Ir, Ni, Pd, Pt. Octahedral metal halides and chalcogenide clusters(M_6X_8 and M_6X_{12} types), chevral phases, triangular clusters and solid state extended arrays, compounds with M-M multiple bonds, major structural types, quadrupole bonds, other bond orders in tetragonal context, relation of clusters to multiple bonds and one dimensional solids.

Nuclear Chemistry:

General characteristics of radioactive decay, decay kinetics, parent daughter decay growth relationships, secular and transient equilibrium, artificial radioactivity, Q value of nuclear reactions, reaction cross-sections, partial and total cross sections, Bohr theory of nuclear reactions, Oppenheimer Phillips process, Photonuclear reactions, thermonuclear reactions, the process of nuclear fission, fission fragments and their mass distribution, charge distribution, fission energy, fission cross sections and thresholds, fission neutrons, high energy fission, neutron evaporation and spallation, radioanalytical techniques and activation analysis.

UNIT-II

Bio-inorganic Chemistry:

Essential and trace elements, importance of metal ions in biological system, biochemistry of iron, Iron storage and transport pigments, metalloporphyrins, mechanism of O_2 binding and transport by haemoglobin and myoglobin, cooperativity in Hb, Bohr effect, other O_2 carrying pigments, hemerythrin and hemocyanin, Cytochromes-structure and function, CN- and CO poisoning, Ferredoxin and rubredoxin. Metalloenzymes: Zn enzymes carboxypeptidase and carbonic anhydrase, Cu enzyme superoxide dismutase, nitrogenases and nitrogen fixation, metal deficiency diseases, toxic effects of metals, chelation therapy, metal complexes in medicine.

Supramolecular Chemistry:

Definition and development of supramolecular chemistry, classification of supramolecular host–guest compounds; receptors, coordination and the lock and key analogy, cooperativity and the chelate effect, preorganisation and complementarity, thermodynamic and kinetic selectivity and discrimination, nature of supramolecular interactions, solvation and hydrophobic effects.

Books Recommended:

1. *Nuclear and Radiations Chemistry,* Fiedelander and Kennedy.
2. *Advanced Inorganic Chemistry,* Cotton and Wilkinson, John Wiley (5th edition and 6th edition).
3. *Inorganic Chemistry,* Shriver and Atkins (4th edition) Oxford University Press.
4. *Nuclear and Radiations Chemistry,* Fiedelander and Kennedy.
5. *Principles of Radio Chemistry*, Indian Association of Nuclear Chemists and Allied Scientists. Editors D.D. Sood, N. Rama moorthy, A.V.R. Reddy.
6. *Essentials of Nuclear Chemistry,* H.J. Arnikar, New Age International Publishers
7. *Nanotechnology, Fundamentals and Applications;* Manasi Karkare, I.K. International Publishing House Pvt. Ltd.
8. *Modern Aspects of Inorganic Chemistry,* H.J. Emeleus and A.G. Sharpe.
9. *Supramolecular Chemistry (Concepts and Perspectives),* Jean Marie Lehn.
10. *Supramolecular Chemistry,* Steed and Atwood.
11. *Bioinorganic and Supramolecular Chemistry,* Ajay Kumar Bhagi and G.R. Chatwal, Himalaya Publishing House

MSCHE 412: INORGANIC CHEMISTRY PRACTICALS-III

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

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

CO1: Determine metal ions spectrophotometrically by complexation with suitable ligands.

CO2: Plot spectra, assign transitions and determine oscillator strengths in the UV- Vis spectra of transition metals.

CO3: Determine the relative position of ligands in spectrochemical series based on 10Dq values.

CO4: Recording the fluorescence spectra of organic dyes and explain fluorescence quenching phenomenon.

CO5: Demonstrate working knowledge of HPLC and GC.

CO6: Synthesise metal and metal oxide nanoparticles.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:

Experiment I: 35 marks

Experiment II: 35 marks

Viva-Voce: 20 marks

Practical Record Book: 10 marks

1. Spectrophotometric analysis
    a) Determination of Fe(II) with 1,10 phenanthroline spectrophotometrically.
    b) Determination of Cu(II) with diethyl dithiocarbamate spectrophotometrically.
    c) Determination of Fe(III) with potassium thiocyanate spectrophotometrically.
    d) Determination of Cr(VI) with diphenylcarbazide spectrophotometrically.
    e) Determination of Ni(II) with dimethylglyoxime spectrophotometrically.

2. To find out oscillator strengths and assignment of d-d bands to transitions in hexaaquo ions of Cr(III), Fe(II), Co(II), Ni(II) and calculate 10 Dq and B for $[Ni(H_2O)_6]^{2+}$.
3. Verification of relative position of following ligands in spectrochemical series: water, pyridine, ammonia, dimethylsulphoxide, acetyl acetonate, ethylenediamine, acetate and urea.
4. To study the quenching phenomenon of organic dye using fluorescence spectroscopy.
5. Demonstration of High-Pressure Liquid Chromatographic and Gas Chromatographic techniques.
6. Synthesis of Nanoparticles of ZnO/ZnS/Ag.

Books recommended:

1. *Vogel's textbook of Quantitative Chemical Analysis,* Pearson Education, 6th edition.
2. *Instrumental Methods of Analysis,* Willard, Hobert H. *et al*: 7th Ed. Wardswor Publishing Company, Belmont, California, USA, 1988.
3. *Physical methods in Inorganic Chemistry*, R.S. Drago.

MSCHE 421: CHEMISTRY OF NATURAL PRODUCTS

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

After the completion of this course student will be able to

CO1: Learn the methods of isolation, purification, and characterization of simple chemical constituents like alkaloids, terpenoids, steroids etc. obtained from the natural sources.

CO2: Explain the importance of natural compounds as leading molecules for new drug discovery.

CO3: Apply the chemical principles highlighted by the study of these natural products to synthesize other unseen natural product structures.

CO4: Learn how biosynthetic pathways can be explored using labelled biosynthetic precursors.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory. Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Studies on Biosynthetic Pathways of Natural Products

The acetate hypothesis, poly-keto acids, their aldol type cyclisations and meta orientations of hydroxyl groups in naturally occurring Phenols. Isoprene rule. Geranyl pyrophosphate and its conversion into α-pinene, thujene and borneol. Fernesyl pyrophosphate, geranyl geranyl

pyrophosphate and mechanistic considerations for their interconversions into cadinene and abietic acid.

Terpenoids and Carotenoids

Classifications, Nomenclature, occurrence, isolation, general methods of structure determination. Biosynthetic approach and synthesis of following molecules: geraniol, α- terpineol, menthol, zingiberene, santonin, abietic acid, camphor, vitamin-A, longifolene, β- carotene (basic structure of α-carotene, γ-carotene also), β-caryophyllene, cedrene, cedrol, Himachalene.

Alkaloids

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, structure, stereochemistry, biosynthesis of Ephedrine, Coniine, Nicotine, Quinine, Morphine, Reserpine.

UNIT-II

Steroids

Occurrence, physiological action, basic skeleton, stereochemistry, structure determination, synthesis of Cholesterol, Bile acids, Testosterone, Androsterone, Progesterone, Estrone. Biosynthesis of steroids.

Carbohydrates

Types of naturally occurring sugars: Deoxy-sugars, amino sugars, branched chain sugars. General method of structure and ring size determination and biosynthesis with particular reference to maltose, lactose, sucrose, pectin, starch and cellulose.

Amino acids, Peptides and Proteins

Introduction, amino acid classification and structure, chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins, forces responsible for holding secondary structures. α-helix and β-sheet. Tertiary structure of protein folding.
Quaternary structure. Biosynthesis of amino acids and proteins.

Books Recommended:

1. *Organic Chemistry,* I.L. Finar; Vol. 1, 2. Pubs: ELBS (1994).
2. *Classics in Total Synthesis,* Nicolaou K.C. and Sorensen E.J.; Pubs: VCH N.Y. (1986).
3. *Biosynthesis of Natural Products,* Manitto P., Pubs: Horwood Ltd. (1981).
4. *Organic Chemistry,* Solomon T.W.G. and Fryhle C.B., 7th Edition, Pubs: John Wiley and sons Ins. N.Y. (2000).

5. *Natural Products – Chemistry and Biological Significance,* J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, Longman, Essex.

MSCHE 422: ORGANIC CHEMISTRY PRACTICALS-III

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

On completion of the course, the student should be able to:
CO1: Know the application of analytical methods based on titrations.
CO2: Understand the principles of chromatography for characterizing amino acids, sugars and dyes.
CO3: Gain an understanding of sampling for absorbance spectrophotometry.
CO4: Utilize UV spectrophotometer to monitor quantitative analysis.
CO5: Understand the performance of graphical analysis to analyze laboratory results.

INSTRUCTIONS

The candidates will perform two experiments. The distribution of marks is as given below:
Experiment I: 35 marks
Experiment II: 35 marks
Viva-Voce: 20 marks
Practical Record Book: 10 marks

1. Quantitative Estimation by Extraction Method

a) To determine percentage purity of sodium benzoate in the given sample by extraction method.
b) To find percentage purity of sodium salicylate by extraction method.

2. Olefinic bond

a) To determine percentage purity of allyl alcohol by addition method using brominating reagent.
b) To find the amount of mesityl oxide using brominating reagent.

3. Diols

a) To determine the percentage purity of given sample of glycol using periodic acid.

b) To determine the amount of glycerol per litre using periodic acid.

4. Chromatography

a) Separation and identification of alkaloids by paper or thin layer chromatography and determination of Rf values.
b) Separation of mixture of glucose, fructose and sucrose by paper chromatography and determination of Rf values.
c) Separation of mixture of glucose, fructose and sucrose by thin layer chromatography and determination of Rf values.
d) Separation of o- and p- nitrophenols by column chromatography.

5. Spectrophotometric (UV/VIS) Estimations

a) Amino Acid
b) Carbohydrate
c) Cholesterol
d) Ascorbic Acid
e) Aspirin
f) Caffeine

NOTE: *Subject to the availability of Instrument/chemicals, the experiments can be substituted by alternate experiments.*

Books Recommended:

1. *Practical Organic Chemistry*, Mann, F.G & Saunders, B.C., Pearson Education.
2. *Practical Organic Chemistry*, Furniss, B.S.; Hannaford, A.J.; Smith, P.W.G. & Tatchell,A.R. 5th Ed. Pearson.
3. *Quantitative Organic Analysis,* Arthur I. Vogel, 2nd Ed. Pearson.

MSCHE 431: Advanced Physical Chemistry -II

Maximum Marks: 100 L T P 5 0 0
Semester Examination: 70 Lectures: 60
Internal Assessment: 30 Time: 3hrs Pass marks: 35%

COURSE OUTCOMES

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

CO1: Explain about the structure and properties of solid crystals.
CO2: Illustrate the principle, instrumentation, and applications of various diffraction methods.
CO3: Explain metal defects and thermodynamics of metal defects, crystal defects, line defects and plane defects.
CO4: Explain about the Electrical Double Layer and its structure, electrokinetic phenomenon, null point, liquid junction potential and Debye Huckel theory. Explain electrocatalysis and kinetics of electrode reactions.

INSTRUCTIONS FOR THE PAPER SETTER

The question paper will consist of three units: I, II, and III. Unit I will have four questions (from the respective unit of syllabus) carrying 10 marks each, Unit II will also have four questions (from the respective unit of syllabus) carrying 10 marks each. Unit III will consist of 10 short answer questions that will cover the entire syllabus and will be of 3 marks each.

INSTRUCTIONS FOR THE CANDIDATES

Candidates are required to attempt two questions each from unit I and II. Unit III is compulsory.
Note: Internal assessment will be given based on mid semester tests (15), attendance (8), and assignments (7).

UNIT-I

Crystallography and X-Rays

Crystallography: Crystals, crystals lattices, unit cell and crystal systems, Bravais lattice, direction and lattice planes, Miller indices, reciprocal lattice, derivation of spacing formula for cubic, tetragonal and orthorhombic crystals, stereographic projections, crystal structure of CsCl, NaCl, diamond, ZnS, CaF_2, point defects, stoichiometric and non-stoichiometric crystal defects, thermodynamics of Schottky and Frenkel defects formation, color centers, line defects and plane defects.

X-Ray Diffraction : X-ray diffraction and the directions of diffracted beam, X-ray spectroscopy, methods of X-ray diffraction-Bragg's method and Laue's method, derivation of Bragg's law and Laue's law from concept of reciprocal lattice, rotating crystal method, powder method, diffraction under non-ideal conditions, the intensities of diffracted beams scattered by an electron, atom and unit cell, the structure factor and its calculations, the factors influencing the intensity of diffracted lines on the powder pattern, determination of crystal structure, electron diffraction scattering by gases, Wierl equation, measurement techniques.

UNIT-II

Electrochemistry: Conductance and Ionic Mobilities: Conductance, Variation of equivalent conductance with concentration, conductance at high frequencies and high potentials, Bjerrum's theory of ion association in electrolyte solutions, ion triplets in electrolyte solutions.
Ions in solution: Deviation from ideal behaviour, ionic activity, mean ionic activity coefficients, ion-ion and ion-solvent interactions, Born model of ion-solvent interaction, Debye-Huckel theory of activity coefficients of strong electrolytes, Debye-Huckel limiting law, verification of Debye-Huckel limiting law, Debye Huckel Onsager equation, modification of Debye Huckel Onsager equation, Applications of conductance measurements: Conductometric titrations, potentiometric titrations.
Applied Electrochemistry: Electrical Double Layer, structure of electrical double layer, parallel plate condenser theory, diffuse layer theory and adsorption theory of double layer, electrokinetic phenomenon, null point and its determination.
Electrocatalysis: Electro catalysis in redox reactions, electro catalysis in reaction involving adsorbed species, some specific features of electro catalysis.
Kinetics of electrode reactions: The Buttler-Volmer equation, equilibrium current density, the diffusion over potential.

Books Recommended:

1. *Elements of X-Ray Diffraction*, B.D. Cullity.
2. *Physical Methods in Chemistry,* R.S. Drago.
3. *Modern Electrochemistry 2A*, John O'M Bockris, Amulya K.N. Reddy and Maria Gamboa-Aldeco, Springer.
4. *An introduction to Electrochemistry*, Samuel Glasstone, Litton Educational Publishing.
5. *Principles of Physical Chemistry,* B.R. Puri, L.R. Sharma & M.S. Pathania, Vishal Publishing Co.
6. *Advanced Physical Chemistry,* J.N. Gurtu and A. Gurtu, Pragati Prakashan.

MSCHE 432: INSTRUMENTAL PHYSICAL CHEMISTRY PRACTICALS

Maximum Marks: 100 L T P 0 0 3.75
Pass marks: 35% Time: 6 hours Lectures: 60

COURSE OUTCOMES

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

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

CO1: Demonstrate the practicals of conductance, pH meter, potentiometer and able to know handling of these instruments.

CO2: Determine the rate of reaction and order of a reaction with the help of a conductometer.

CO3: Determine degree of hydrolysis of the salts with these instruments.

CO4: Evaluate the dissociation constant of week electrolyte.

CO5: Analyze and interpret the data collected by the instruments discussed in the course.

(I) Conductance Measurements

1. To determine the order of reaction of the saponification of ethyl acetate by sodium hydroxide.
2. To verify Ostwald dilution law for a given weak electrolyte and determine its dissociation constant.
3. To verify Walden Rule.
4. To determine solubility of lead sulphate.
5. To determine degree of hydrolysis of the salts.
6. To determine the strength and composition of the solution of HCl , CH_3COOH and $CuSO_4$ by titrating it against NaOH.
7. To follow the titration of aqueous solution of potassium chloride against silver nitrate solution.
8. To determine CMC of a surfactant.
9. To study the kinetics of hydrolysis of tert. butyl chloride by conductance measurement.
10. To verify Debye-Huckel Onsager equation.

(II) pH Measurements

1. To determine the strength and composition of the solution of HCl and CH_3COOH by titrating it against NaOH.
2. To determine dissociation constant of weak acid and weak base.
3. To determine buffer capacity of the given buffer solution.
4. To determine degree of hydrolysis of the salts of weak acids and strong bases and that of strong acids and weak bases.

(III) Potentiometry

1. To find the strength of mixture of halides by titrating it against silver nitrate solution.
2. To determine the composition of zinc ferrocyanide complex.
3. To determine the strength of HCl and CH_3COOH solution by titrating it against NaOH.
4. To determine the dissociation constant of CH_3COOH.
5. To determine the concentration of a reductant or an oxidant.
6. Determination of the solubility of the sparingly soluble salts.

Books Recommended:

1. Advanced Physical Chemistry Experiments, Gurtu-Gurtu:.
2. Senior Practical Physical Chemistry, B.D.Khosla V.C Garg & Adarsh Gulati:
3. Practical Physical Chemistry, B.Viswanathan & P.S Raghavan :.
4. Practical Physical Chemistry, A.M. James and F. E. Prichard, Longman
5. Practical Physical Chemistry, Alexander, and Findley.
6. Advanced Practical Chemistry, Jagdamba Singh, R.K.P Singh, Jaya Singh.
7. Advanced Practical Chemistry, R.Mukhopadhyay and P. Chatterjee.
8. University Practical Chemistry, P.C. Kamboj.
9. Advance Practical Physical Chemistry, J. B.Yadav.
10. Textbook of Chemistry Practical, Bidhan Chandra Ray and Satyanarayan Das:

MSCHE 405: INDUSTRIAL TRAINING

Maximum Marks: 50 L T P 0 0 2
Pass marks: 35% Time: 6 hours

COURSE OUTCOMES

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

CO1: Understand the actual working environment of industry.

CO2: Apply the acquired knowledge in real work environment.

CO2: Develop work habits and attitudes necessary for job success.

CO3: Develop written communication and technical report writing skills.

The candidates will be required to undergo training in academic/analytical labs or industries and will submit a project report followed by its presentation. Candidates will be awarded credits for the project report and training based on their presentation and viva voce.