

# Indira Gandhi University Meerpur Rewari



**Examination Scheme  
&  
Syllabi  
for  
M.Sc. Chemistry  
(SEMESTER- I & IV)**



**INDIRA GANDHI UNIVERSITY, MEERPUR, REWARI**  
**Scheme of Examination for M.Sc. Chemistry**

**Semester-I**

**Credits = 31**

**Marks = 700**

Paper Code	Subjects	Type of Course	Contact Hours Per Week			Credits			Examination Scheme			Total
			Theory	Practical	Total	Theory	Practical	Total	Theory	Internal Assessment	Practical	
CHE-101	Inorganic Chemistry-I (Chemistry of Transition Metals)	C.C	04	--	04	04	--	04	80	20		100
CHE-102	Physical Chemistry-I (Principles of Physical Chemistry)	C.C	04	--	04	04	--	04	80	20		100
CHE-103	Organic Chemistry-I (Conceptual Organic Chemistry & Stereochemistry)	C.C	04	--	04	04	--	04	80	20		100
<b>Discipline Centric Elective Course (Any Two)</b>												
CHE-104	Biology for Chemists & Mathematics for Chemists	DCEC	04	--	04	04	--	04	80	20		100
CHE-105	Statistical Techniques & Its Applications	DCEC	04	--	04	04	--	04	80	20		100
CHE-106	Sustainable and Green Chemistry	DCEC	04	--	04	04	--	04	80	20		100
CHE-107	Practical-I Inorganic Chemistry	C.C	--	02X03	06	--	03	03	-		50	50
CHE-108	Practical-II Physical Chemistry	C.C	--	02X03	06	--	03	03	-		50	50
CHE-109	Practical-III Organic Chemistry	C.C		02X03	06		03	03			50	50
CHE-110	Seminar		--	--	01	-	-	01	-		-	25
CHE-111	Self Study Paper		--	--	01	-	-	01	-		-	25

<b>Total</b>	<b>20</b>	<b>18</b>	<b>40</b>	<b>20</b>	<b>09</b>	<b>31</b>	<b>400</b>	<b>100</b>	<b>150</b>	<b>700</b>
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**CC = Core Course**

**DCEC = Discipline Centric Elective Course**

**FEC=Foundation Elective Course**

**Scheme of Examination for M.Sc. Chemistry**
**Semester-II**
**Credits = 33**
**Marks = 750**

Paper Code	Subjects	Type of Course	Contact Hours Per Week			Credits			Examination Scheme			Total
			Theory	Practical	Total	Theory	Practical	Total	Theory	Internal Assessment	Practical	
CHE-201	Inorganic Chemistry-II (Organometallic Chemistry & Molecular Clusters)	CC	04	--	04	04	--	04	80	20		100
CHE-202	Physical Chemistry-II (Physical Chemistry: Concepts & Applications)	CC	04	--	04	04	--	04	80	20		100
CHE-203	Organic Chemistry-II (Organic Reaction Mechanism)	CC	04	--	04	04	--	04	80	20		100
<b>Discipline Centric Elective Course (Any Two)</b>												
CHE-204	Supramolecular & Photochemistry	DCEC	04	--	04	04	--	04	80	20		100
CHE-205	Group Theory & Molecular Spectroscopy	DCEC	04	--	04	04	--	04	80	20		100
CHE-206	Organic Chemistry of Polymers	DCEC	04	--	04	04	--	04	80	20		100
CHE-207	Communication Skills & Personality Development	FEC	02	--	02	02	--	02	40	10		50
CHE-208	Practical-I Inorganic Chemistry	C.C	-	02×03	06	--	03	03	-		50	50
CHE-209	Practical-II Physical Chemistry	C.C	-	02×03	06	--	03	03	-		50	50
CHE-210	Practical-III Organic Chemistry	C.C		02×03	06		03	03				
CHE-211	Seminar		-	-	01	-	-	01	-		-	25

CHE-212	Self Study Paper		-	-	01	-	-	01	-		-	25
<b>Total</b>			<b>22</b>	<b>18</b>	<b>42</b>	<b>22</b>	<b>09</b>	<b>33</b>	<b>440</b>	<b>110</b>	<b>150</b>	<b>750</b>

**CC = Core Course**

**DCEC = Discipline Centric Elective Course**

**FEC = Foundation Elective Course**

## Scheme of Examination for M.Sc. Chemistry

## Semester-III

Credits = 34

Marks = 800

Paper Code	Subjects	Type of Course	Contact Hours Per Week			Credits			Examination Scheme			Total
			Theory	Practical	Total	Theory	Practical	Total	Theory	Internal Assessment	Practical	
CHE-301	Organic Spectroscopy	C.C	04		04	04		04	80	20		100
CHE-302	Inorganic Spectroscopy	C.C	04		04	04		04	80	20		100
CHE-303	Analytical Chemistry	C.C	04		04	04		04	80	20		100
CHE-304(a) CHE-304(b) CHE-304(c)	Inorganic special-I Physical Special-I Organic Special-I	C.C	04		04	04		04	80	20		100
CHE-305(a) CHE-305(a) CHE-305(a)	Inorganic special-II Physical Special-II Organic Special-II	C.C	04		04	04		04	80	20		100
<b>Open Elective Course</b>												
CHE-306	To be chosen from the pools of open electives provided by the other departments of University	OEC	03		03			03	80	20		100
CHE-307	Practical-I Inorganic Chemistry/ Physical Chemistry/ Organic Chemistry	C.C	-	02X03	06	--	03	03	-		50	50
CHE-308	Practical-II Inorganic Chemistry/ Physical Chemistry/ Organic Chemistry	C.C	-	02X03	06	--	03	03	-		50	50
CHE-309	Practical-III Inorganic Chemistry/ Physical Chemistry/	C.C		02X03	06	--	03	03			50	50

	Organic Chemistry											
CHE-310	Seminar		--	--		-	-	01	-		-	25
CHE-311	Self Study Paper		--	--		-	-	01	-		-	25
<b>Total</b>			<b>23</b>	<b>18</b>	<b>41</b>	<b>20</b>	<b>09</b>	<b>34</b>	<b>480</b>	<b>120</b>	<b>150</b>	<b>800</b>

CC = Core Course

DCEC = Discipline Centric Elective Course

OEC = Open Elective Course



## Scheme of Examination for M.Sc. CHEMISTRY

Semester-IV

Credits = 31

Marks = 700

Paper Code	Subjects	Type of Course	Contact Hours Per Week			Credits			Examination Scheme			Total
			Theory	Practical	Total	Theory	Practical	Total	Theory	Internal Assessment	Practical	
CHE-401(a) CHE-401(b) CHE-401(c)	Inorganic special-III Physical Special-III Organic Special-III	C.C	04		04	04		04	80	20		100
CHE-402(a) CHE-402(b) CHE-402(c)	Inorganic special-IV Physical Special-IV Organic Special-IV	C.C	04		04	04		04	80	20		100
CHE-403(a) CHE-403(b) CHE-403(c)	Inorganic special-V Physical Special-V Organic Special-V	C.C	04		04	04		04	80	20		100
CHE-404(a) CHE-404(b) CHE-404(c)	Inorganic special-VI Physical Special-VI Organic Special-VI	C.C	04		04	04		04	80	20		100
CHE-405	Computational Chemistry	C.C	04		04	04		04	60	40		100
CHE-406	<b>Practical-IV</b> Inorganic Chemistry/ Physical Chemistry/ Organic Chemistry	C.C	-	02X03	06	--	03	03	-		50	50

CHE-407	<b>Practical-V</b> Inorganic Chemistry/ Physical Chemistry/ Organic Chemistry	C.C	-	02X03	06	--	03	03	-		50	50
CHE-408	<b>Practical-VI</b> Inorganic Chemistry/ Physical Chemistry/ Organic Chemistry	C.C		02X03	06	--	03	03			50	50
CHE-409	Seminar		-	-		-	-	01	-		-	25
CHE-410	Self Study Paper		-	-		-	-	01	-		-	25
<b>Total</b>			<b>20</b>	<b>18</b>	<b>38</b>	<b>20</b>	<b>09</b>	<b>31</b>	<b>380</b>	<b>120</b>	<b>150</b>	<b>700</b>

CC = Core Course      DCEC= Discipline Centric Elective Course  
Duration: 02 Years      Total Credits = 129      Total Marks = 2950

**Indira Gandhi University Meerpur Rewari****M.Sc- Chemistry****General Instructions****1. Seminar/ Journal Club**

Max.Marks-25

Every candidate will have to deliver a seminar of 30 minutes duration on a topic (not from the syllabus) which will be chosen by him / her in consultation with the teacher of the department. The seminar will be delivered before the students and teachers of the department. A three member committee (one coordinator and two teachers of the department of different branches) duly approved by the departmental council will be constituted to evaluate the seminar. The following factors will be taken into consideration while evaluating the candidate. Distribution of marks will be as follows:

- |                                |          |
|--------------------------------|----------|
| 1. Presentation                | 10 marks |
| 2. Depth of the subject matter | 10 marks |
| 3. Answers to the questions    | 05 marks |

**2. Self Study Paper**

Max.Marks-25

**Objective:** This course intends to create habits of reading books and to develop writing skills in a manner of creativity and originality. The students are to emphasis his/her own ideas/words which he/she has learnt from different books, journals and newspapers and deliberate the same by adopting different ways of communication techniques and adopting time scheduling techniques in their respective fields. This course aims:

- To motivate the students for innovative, research and analytical work
- To inculcate the habit of self study and comprehension
- To infuse the sense of historical back ground of the problems
- To assess intensity of originality and creativity of the students

Students are guided to select topic of their own interest in the given area in consultation with their teachers/Incharge/Resource Person.

**Instructions for Students**

1. Choose the topic of your interest in the given areas and if necessary, seek the help of your teacher.
2. Select a suitable title for your paper.
3. You are expected to be creative and original in your approach.
4. Submit your paper in two typed copies of A4 size 5-6 pages (both sides in 1.5 line spaces in Times New Roman Font size 12).

5. Organize your paper in three broad steps:
  - (a) Introductions
  - (b) Main Body
  - (c) Conclusion
6. Use headings and sub-headings
7. Use graphics wherever necessary
8. Give a list of books/references cited/used
9. The external examiner will evaluate the self-study paper in two ways i.e. Evaluation 15 Marks and Viva-Voce 10 marks.

### **Distribution of Marks**

- |           |   |                 |
|-----------|---|-----------------|
| <b>1.</b> | The evaluation is divided into different segment as under : | <b>15 Marks</b> |
| (i)       | Selection of Topic  | - 3 Marks       |
| (ii)      | Logical Organization of subject matter                      | - 5 Marks       |
| (iii)     | Conclusions   | - 5 Marks       |
| (iv)      | References  | - 2 Marks       |
| <b>2.</b> | Viva-Voce:  | <b>10 Marks</b> |

The external examiner will hold Viva-Voce based on contents of the student's Self Study Paper focusing upon the description by the Candidate.

**M.Sc-Chemistry**  
**Semester-I**

**CHE I01: Inorganic Chemistry-I**  
**(Chemistry of Transition Metals)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Transition Metal Chemistry : Structure, bonding and properties of transition metal ligand complexes—ligand, coordination, geometry, isomerism (recapitulation); thermodynamic stability, successive and overall stability constants and their interactions, trends in stepwise constants, factors affecting stability of metal complexes with reference to the nature of metal ion and ligand, Irving-William series, chelate and macrocyclic effect, thermodynamic origin of chelate effect, determination of binary formation constants by pH-metry and spectrophotometry.

Theories of Bonding- Crystal field theory and its limitation; d-orbital splitting in octahedral, square planar, square pyramidal and trigonal bipyramidal complexes, John-Teller distortion, Molecular orbital theory of octahedral, tetrahedral and square planar complexes (with and without  $\pi$ -bonding).

**Unit-II**

Electronic spectra and magnetic properties: Electronic arrangements of microstates, calculation of the number of microstates in various electronic arrangements, spectroscopic term symbols and splitting of terms in free atoms, determining the ground state terms, correlation and spin-orbit coupling in free ions for 1st series of transition metals. Interpretation of electronic spectra; Orgel and Tanabe-Sugano diagrams for transition metal complexes ( $d^1 - d^9$  states), Spectrochemical and nephelauxetic series, calculation of  $Dq$ ,  $B$ ,  $\beta$  parameters, charge transfer spectra, magnetic properties; anomalous magnetic moments, magnetic exchange coupling and spin crossover.

**Unit-III**

Reaction Mechanisms-I : Inert and labile complexes, kinetic application of valence bond and crystal field theories, substitution reactions in octahedral complexes- acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, water exchange, anation reactions, reactions without metal ligand bond cleavage, racemization of tris-chelate complexes, electrophilic attack on ligands.

**Unit-IV**

Reaction Mechanisms-II: Substitution reactions in square planar complexes, the trans effect, theories of trans effect, redox reactions, mechanism of electron transfer reactions – types; outer sphere electron

transfer reactions, cross reactions and Marcus-Hush theory, and inner sphere electron transfer mechanism, electron exchange, metal ion catalysed reactions, mixed valence complexes and their electron transfer.

**Suggested Readings:**

1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry: Principles of Structure and Reactivity, J.E. Huhey, E.A. Keiter and R.L. Keiter, Pearson Education.
3. Shriver & Atkins: Inorganic Chemistry, P.W. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, Oxford University Press.
4. Chemistry of the Elements, N.N. Greenwood and A. Earnshaw, Pergamon.
5. The Chemical bond, J.N.Murrel, SFA Kettle and JM. Tedder; Wiley, New York.
6. Modern Aspects of Inorganic Chemistry, H.J. Emeleus and Sharpe.
7. Concepts and Models of Inorganic Chemistry, B. Douglas, D.H. McDaniel and J.J.Alexander; John Wiley and Sons.
8. Inorganic Chemistry, A Modern Introduction, T Moller, John Wiley and Sons.
9. Mechanism of Inorganic Reactions, F. Basolo and R.G. Pearson, John Wiley and Sons, New York.
10. Inorganic Reaction Mechanism, M.L. Tobe; Nelson, Wlaton and Thames
11. Coordination Chemistry, Banerjea; Tata McGraw Hill.

**M.Sc-Chemistry**  
**Semester-I**

**CHE I02: Physical Chemistry-I**  
**(Principles of Physical Chemistry)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Thermodynamics: Brief resume of first and second Law of thermodynamics. Entropy changes in reversible and irreversible processes; variation of entropy with temperature, pressure and volume, entropy concept as a measure of unavailable energy and criteria for the spontaneity of reaction, free energy functions and their significance, criteria for spontaneity of a process, partial molar quantities (free energy, volume, heat concept), Gibb's-Duhem equation, variation of chemical potential with temperature and pressure, chemical potential for an ideal gas, chemical potential in ideal gas mixture, determination of partial molar volume, thermodynamic functions of mixing (free energy, entropy, volume and enthalpy), concept of escaping tendency and chemical potential.

**Unit-II**

Chemical Dynamics: Effect of temperature on reaction rates, Unimolecular reactions, Lindemann-Hinshelwood mechanism of unimolecular reactions. Rate law for opposing reactions of I<sup>st</sup> order and II<sup>nd</sup> order, Rate law for consecutive I<sup>st</sup> order reactions, Collision theory of reaction rates and its limitations, steric factor, Arrhenius equation and activated complex theory, the comparison of collision and activated complex theory, chain reactions (hydrogen-halogen) reaction.

**Unit-III**

Electrochemistry: Debye -Huckel theory of ion- ion interactions: potential and excess charge density as a function of distance from the central ion, Debye Huckel reciprocal length, ionic cloud and its contribution to the total potential. Applicability and limitations of Debye-Hückel limiting law, activity coefficient, Physical significance of activity coefficients, mean activity coefficient of an electrolyte, Debye - Huckel-Onsager treatment for aqueous solutions and non-aqueous solutions, Debye -Falkenhagen effect, Wein effect, D-H-O equation's limitations.

Metal/Electrolyte interface, Concept of electrical double layer and its structure: Helmholtz-Perrin, Gouy-Chapman, and Stern models, electrokinetic phenomena.

### Unit-IV

Quantum Mechanics: Postulates of Quantum Mechanics, Quantum mechanical operators and their commutations relation, Heisenberg's Uncertainty Principle, Hermitian operators, (elementary ideas, quantum mechanical operator for linear momentum and angular momentum). The average value of the square of Hermitian operators, commuting operators and uncertainty principle ( $x$  &  $p$ ), derivation of Schrodinger wave equation, eigen function and eigen values, Schrodinger wave equation for a particle in one dimensional box, evaluation of average position, average momentum and determination of uncertainty in position and momentum and hence Heisenberg's uncertainty principle, pictorial representation of the wave equation of a particle in one dimensional box and its influence on the kinetic energy of the particle in each successive quantum level, lowest energy of the particle, Schrodinger wave equation for a particle in a three dimensional box and the concept of degeneracy of energy levels.

#### Suggested Readings:

1. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
2. Quantum Chemistry, I.M. Levine, Prentice Hall.
3. Quantum Chemistry, B. K. Sen, Kalyani Publishers
4. Quantum Chemistry, R. Prasad, New Age International.
5. An Introduction to Chemical Thermodynamics, R.P. Rastogi and R.R. Misra, Vikas Pub.
6. Physical Chemistry, P.W. Atkins, Oxford University Press.
7. Thermodynamics for Chemists, S. Glasstone, Affiliated East -West Press.
8. Thermodynamics, I.M. Klotz and R.M. Rosenbers, Benzamin.
9. Chemical Kinetics, K.J. Laidler, McGraw Hill.
10. Kinetics and Mechanism, A. A. Frost and R.G. Pearson, John Wiley and Sons.
11. Electrochemistry, S. Glasstone, Affiliated East -West Press.
12. Physical Chemistry, G.W. Castellan, Narosa.



**M.Sc-Chemistry**  
**Semester-I**

**CHE 103: Organic Chemistry-I**  
**(Conceptual Organic Chemistry & Stereochemistry)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Nature of Bonding in Organic molecules: Delocalized chemical bonding –conjugation, cross conjugation, resonance, tautomerism. Concept of aromaticity; Huckel’s rule, energy level of  $\pi$ -molecular orbitals, annulenes, antiaromaticity, homo-aromaticity. anti- and homo-aromatic systems. Bonds weaker than covalent, addition compounds.

Reaction Mechanism: Structure and Reactivity: Types of mechanisms, types of reactions, Relationship between thermodynamic stability and rates of reactions - kinetic versus thermodynamic control of product formation – Hammond postulate. Potential energy diagrams, transition states and intermediates, methods of determining mechanisms, guide lines for proposing reaction mechanism. The Hammett equation and linear free energy relationship, substituent and reaction constants. Generation, structure, stability and reactivity of reactive intermediates, carbocations, carbonanions, Free Radicals, Carbenes, Nitrenes.

**Unit-II**

Stereochemistry-I: Introduction to molecular symmetry and chirality – examples from common objects to molecules – axis, plane, center, alternating axis of symmetry. D-L, R-S, E-Z and threo-erythro nomenclature, interconversion of Fischer, Newman, Sawhorse and flying wedge formulae. Conformational analysis, enantiomerism and diastereomerism of simple acyclic, cyclic system (chair and boat configuration) and fused and bridged bicyclic systems (decalins). Conformation and reactivity some examples, chemical consequence of conformational equilibrium - Curtin-Hammett principle. Axial and planar chirality, optical isomerism in allenes, biphenyls (atropoisomerism), spiranes, hemispiranes. Elementary ideas about stereochemistry of tertiary amines, quaternary salts, sulphur and phosphorous compounds.

**Unit-III**

Stereochemistry-II: Topicity of ligands and faces, their nomenclature and prostereoisomerism, stereogenecity, chirogenicity, pseudoasymmetry and prochiral centre. stereospecific and stereoselective reaction. Elementary idea of principle categories of asymmetric synthesis, Cram’s rule and its modification, Prelog rule and horeaus rule. Stereochemistry of sugars- conformations of hexoses, pentoses. Homomorphous sugars, abnormal mutarotation and  $\Delta$ -2 instability factor. Stereochemistry of

decalins, Chemical correlation of configuration-determination of relative configuration of 2-butanol, isoserine, alanine, malic acid, lactic acid and mandelic acid.

#### Unit-IV

Aliphatic Nucleophilic Substitution: The SN<sub>2</sub>, SN<sub>1</sub>, mixed SN<sub>1</sub> and SN<sub>2</sub> SN<sub>i</sub>, SN<sub>1</sub>' , SN<sub>2</sub>' SN<sub>i</sub>' and SET mechanisms. The neighbouring group mechanisms, neighbouring group participation by p and s bonds, anchimeric assistance. Classical and nonclassical carbocations, phenonium ions, common carbocation rearrangements. Application of NMR spectroscopy in the detection of carbocations. Reactivity- effects of substrate structure, attacking nucleophile, leaving group and reaction medium.. Ambident nucleophile, regioselectivity. Phase transfer catalysis.

Aliphatic Electrophilic Substitution: Bimolecular mechanisms - SE<sub>2</sub> and SE<sub>i</sub>. The SE<sub>1</sub> mechanism, Electrophilic substitution accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

#### Suggested Readings:

1. Advanced Organic Chemistry Reactions, Mechanism and Structure, Jerry March, John Wiley.
2. Advanced Organic Chemistry, F. A. Carey and R. J. Sundberg, Plenum.
3. A Guide Book 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. Principles of Organic Synthesis, R. O. C. Norman and J. M. Coxon, Blackie Academic & Professional.
8. Reaction Mechanism in Organic Chemistry, Om Prakash and S. P. Singh, Trinity.
9. Stereochemistry of Organic Compounds, E. L. Eliel and S. H. Wilen, John Wiley & Sons, New York, 1994
10. Stereochemistry of Organic Compounds, D. Nasipuri, New Age International.
11. Stereochemistry of Organic Compounds, P.S, Kalsi, New Age International.
12. Modern methods of Organic Synthesis, W. Carruthers and I. Coldham, First South Asian Edition 2005, Cambridge University Press.
13. Organic Stereochemistry, Robinson M.J. T., Oxford University Press, 2005.
14. Reactive Intermediates in Organic chemistry Issacs N. S, John Wiley
15. Why Chemical Reactions Happen (Paperback), by Keeler J. and Wothers P., Oxford University Press, 2003.

**M.Sc- Chemistry**  
**Semester-I**

**CHE-104**  
**Biology for Chemists**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Cell Biology: Discovery of cell, Structure of Prokaryotic and Eukaryotic cells, classification of cell types, comparison of plant and animal cells, Cell cycle: mitosis & meiosis, Cellular organization: Biomembranes, Fluid mosaic model of membrane structure, cytoplasmic organelles and their functions. Overview of metabolic processes - catabolism and anabolism. ATP - the biological energy currency.

**Unit-II**

Cellular macromolecules: Essential Amino acids and Isoelectric pH, chemical and enzymatic hydrolysis of proteins to peptides, Secondary structure of proteins,  $\alpha$  -helix,  $\beta$ -sheets, triple helix structure of collagen, Quaternary structure, denaturation of proteins.

Carbohydrates; Structure and biological functions of monosaccharides-- glucose, fructose and galactose, disaccharides- sucrose, lactose and maltose. Structural polysaccharides - cellulose and chitin. Storage polysaccharides - starch and glycogen.

Lipids; Fatty acids, essential fatty acids,  $\beta$ -oxidation of fatty acids.

**Unit-III**

Structure of nucleotides, nucleosides, DNA (Watson-Crick model) RNA structure & conformation, Replication of DNA (semi-conservative, conservative and dispersive replication Maselson-Stahl experiment), transcription, translation of genetic material, genetic code, universality of the code, codon, anticodon pairing, RNA, protein biosynthesis (initiation, elongation, termination and processing of the peptide chain).

**Unit-IV**

Oxygen carriers: Porphyrins, metalloporphyrins, Hemoproteins, structure and functions of hemoglobin and myoglobin, Photosynthesis and chlorophyll.

Atmosphere: Chemical composition of atmosphere, atmospheric structure, Earth's radiation balance; oxides of N,C,S and their effects, Green house effect, acid rain, photochemical smog, depletion of ozone.

**Suggested Readings:**

1. Essential Cell Biology by Bruce Alberts, Dennis Bray, Karen Hopkin, and Alexander D Johnson (Hardcover - Mar. 27, 2009).
2. Molecular Biology of the Cell by Bruce Alberts, Alexander Johnson, Julian Lewis, and Martin Raff.
3. Molecular Biology of the Gene (6th Edition) by James D. Watson, Tania A. Baker, Stephen P. Bell, and Alexander Gann.
4. Lehninger Principles of Biochemistry, Fourth Edition by David L. Nelson (Author), Michael M. Cox.
5. Fundamentals of General Organic and Biological Chemistry (Study Guide) by John McMurry (Paperback - Jan. 1999).
6. Environment, Problems and Solutions, D.K.Asthana and Meera Asthana, S.Chand and Co.(2006)
7. Text Book on Environmental Chemistry, Balaram Pani, I.K.International Publishing House(2007)

**M.Sc- Chemistry**  
**Semester-I**

**CHE-104****Mathematics for Chemists**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Vectors: Examples of scalar and vectors, definitions of vectors in two, three spaces, representation and simple properties of vectors, addition and subtraction of vectors, vector addition by the method of triangles, resolution of vectors into rectangular components, addition of vectors by components, multiplication and differentiation of vectors. Scalar product of vectors, vector product, concept of normalization, orthogonality and complete set of unit vectors. Illustration of applications to spectroscopy and quantum chemistry.

Matrices and Determinants: Definition of matrix, types of matrices, viz . row matrix, column matrix, null matrix, square matrix, diagonal matrix, addition, subtraction and multiplication by a number, matrix multiplication. Transpose and adjoint of matrix, elementary transformation, representation and applications (without development of theory) to solution of linear equations. Definition of determinant, properties of determinants, evaluation of determinants. Illustration or applications to group theory, problems in chemistry.

**Unit-II**

Logarithm: Need for logarithm in chemistry. Theory and application of logarithms for solving general and chemical problems.

Graphical Representation of Equations: Rectangular coordinates, straight lines, slope and intercept of the equation, slope and point equation, two point equation, parallel lines, points of intersection, distance between two points, change of origin. Examples from problems in chemistry.

Elements of Algebraic and Trigonometric Functions: The binomial expansion, some example from chemistry, sines, cosines and tangents, trigonometric identities, polar coordinates in trigonometric functions.

**Unit-III**

Differential Calculus: Theory, rules of differentiation, powers, added and subtracted functions, constants, products, quotients, functions of a function, logarithmic differentiation, and parametric functions. Algebraic simplification, differentiation of implicit functions, graphical significance of differentiation, rate of change of slope, successive differentiation. Examples related to maximally populated rotational

energy levels, Bohr's radius and most probable velocity from Maxwell's distribution. Exact and inexact differential with their application to thermodynamic principles.

Partial Differentiation: Partial differentiation, successive partial differentiation. Integral transforms (Fourier and Laplace). Reduction formulae, application to chemical problems. Methods of Lagrangian multipliers, Sterling's approximation, probability theory.

#### **Unit-IV**

Integral Calculus: Integral theory, rules of integration between limits, significance of  $e^x$  exponential equations, methods of integration, viz. algebraic simplifications, substitution, integration by parts, integration by partial fractions, coordinate transformation (e.g., cartesian to spherical polar).

Illustration of application in chemistry. Evaluation of standard integrals used in chemistry.

Differential Equation: Simple differential equations, separable variables, homogeneous equations, exact equations, linear equations, equation of the first and second order, partial differential equation, application to physico-chemical problems.

#### **Suggested Readings:**

1. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill.
2. Mathematical Preparation for General Physics, J.B. Marian, R.C. Davidson Saunder Company.
3. Mathematical Methods for Science Students, G. Stephemen, ELBS.
4. Chemical Thermodynamics, R.C. Reid.

**M.Sc- Chemistry**  
**Semester-I**

**CHE-105**  
**Statistical Techniques & its Applications**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Random Experiment, Sample Space, Events – Simple, Composite, Mutually Exclusive and Exhaustive Events, Various Definitions of Probability, Properties of probability function, Addition Theorem, Conditional Probability, Multiplication Theorem, Baye's Theorem, Independence of Events. Random Variables and Distribution Functions and properties;

**Unit-II**

Measures of Central Tendency: Mean, median and Mode. Measures of Dispersion: Range, Variance, Standard Deviation, Moments, Skewness and Kurtosis  
Probability distributions: Binomial, Poisson, Normal, Gamma, Exponential, Log-Normal.  
Sampling Distributions: Chi-Square, Student's t and F-distributions; their Properties and Applications. Elementary Ideas of Non-Central Distributions.

**Unit-III**

Testing of Hypotheses, Simple and Composite Hypotheses, Null and Alternative Hypotheses, Two Types of Errors, Critical Reason, Level of Significance, Power of the Test, Unbiased Tests, Critical Reason. Maximum Likelihood Ratio Test, Interval Estimation: Method of obtaining Confidence intervals based on Small and Large Samples, Analysis of Variance and Covariance.

**Unit-IV**

Non Parametric Tests: Ordinary Sign Test, Wilcoxon Signed Ranked Test, Goodness of Fit Problem: Chi-Square Test and Kolmogrov – Smirnov One Sample Test, and their Comparison. Two Sample Problems: K-S Two Sample Test, Wald – Wolfowitz Run Test, Mann –Whitney U Test.  
Least-squares fitting: Linear, Polynomial, arbitrary functions: with descriptions of specific methods.  
Correlation and Regression

**Suggested Readings:**

1. Statistics: A Guide to the Use of Statistical Methods in the Physical Sciences, R.J. Barlow, John Wiley, 1989.
2. The Statistical Analysis of Experimental Data, John Mandel, Dover Publications, 1984.
3. Data Reduction and Error Analysis for the Physical Sciences, 3rd Edition, Philip Bevington and Keith Robinson, McGraw Hill, 2003.





**M.Sc- Chemistry**  
**CHE-106**

**Semester-I**

**Green and Sustainable Chemistry**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

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**UNIT-I: Principles and concepts of Green chemistry**

Chemistry in the context of sustainable development, Current status and future perspective. The twelve principles of Green Chemistry.

**UNIT-II: Catalysis and Renewable raw materials**

Introduction to catalysis. Homogeneous and Heterogeneous catalysis, Phase-transfer catalysis and Biocatalysis. Chemical products based on renewable sources.

**UNIT-III: Alternative solvents**

Volatile organic compounds (VOCs) Supercritical fluids. Alternatives in extraction and chromatography. Ionic liquids as solvents: its types, properties and applications.

**UNIT-IV: Green technology and sources of alternative energy**

Photochemical and Electrochemical reactions. Reactions under Microwave, sonication and ball milling. Flow techniques.

**Books suggested**

1. S. E. Manahan, Fundamentals of Environmental Chemistry, 3<sup>rd</sup> ed. (2009) CRC Press.
2. R. A. Sheldon, I. Arends and U. Hanefeld, Green Chemistry and Catalysis, 1<sup>st</sup> ed. (2007) Wiley-VCH.
3. V. K. Ahluwalia and M. Kidwai, New Trends in Green Chemistry, 1<sup>st</sup> ed. (2004) Springer.

4. T. Clifford, Fundamentals of Supercritical Fluids, 1<sup>st</sup> ed. (1999) Oxford press.
5. C. -J. Li, T. -K. Chan, Organic Reactions in Aqueous Media, 1<sup>st</sup> ed. (1997) Wiley- Interscience, Newyork.
6. Recent review articles relevant to above topics (reprints to be handed over to students).

**M.Sc- Chemistry**  
**Semester-I**

**CHE-107 Practical – I**  
**Inorganic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Qualitative Analysis:
  - a) Less common metal ions- Tl, Se, Te, Mo, W, Ti, Zr &V
  - b) Insolubles- Oxides ( $\text{Al}_2\text{O}_3$ ,  $\text{Cr}_2\text{O}_3$ ,  $\text{SnO}_2$ ,  $\text{TiO}_2$ ,  $\text{SiO}_2$ );  
Sulphates (Lead Sulphate, Barium Sulphate Strontium Sulphate and Calcium Sulphate); Halides ( $\text{CaF}_2$ ,  $\text{AgCl}$ ,  $\text{AgBr}$ ,  $\text{AgI}$ )  
\*(2 less common metal ions and 1 insoluble to be given) (30 Marks)
2. Quantitative Analysis:  
Determination of Ferrous, Oxalate, Nitrite etc. by Cerimetry (10 Marks)
3. Viva-Voce (05 Marks)
4. Note Book (05 Marks)

**Suggested Readings:**

1. A Text Book of Macro and Semi-micro Quantitative Analysis, A.I.Vogel, Orient Longman.
2. A Vogel's Text Book of Quantitative Inorganic Analysis, J. Bassett, R.C. Denney, G.B. Jaffery and J. Menaham, Longman, London.

**M.Sc- Chemistry**  
**Semester-I**

**CHE-108 Practical – II**  
**Physical Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Viscosity
    - (i) Determine the viscosity of methyl acetate and ethyl acetate using Ostwald viscometer.
    - (ii) Study the variation of viscosity with concentration for a glycerol solution using Ostwald viscometer and thereafter determine the concentration of unknown solution of glycerol.
    - (iii) Determine the molar mass of a polymer.
  2. Conductometry
    - (i) Determine the strength of strong acid/ weak acid by conductometric titration with strong base.
    - (ii) Determine the strength of strong acid and weak acid in a mixture by conductometric titration with strong base.
    - (iii) Study precipitation titration between KCl and AgNO<sub>3</sub> conductometrically. Determine the strength of given solution of AgNO<sub>3</sub>.
  3. Distribution Law
    - (i) Determine the distribution coefficient of benzoic acid between benzene and water.
    - (ii) Determine the distribution coefficient of iodine between carbon tetrachloride and water.
    - (iii) Determine distribution coefficient of ammonia between chloroform and water.
  4. Adsorption
    - (i) Verify the Freundlich and Langmuir adsorption isotherms for adsorption of acetic acid on activated charcoal.
    - (ii) Verify the Freundlich and Langmuir adsorption isotherms for adsorption of oxalic acid on activated charcoal.
- \*Two Experiments 2x20 = 40 Marks
5. Viva-Voce (05 Marks)
  6. Note-Book (05 Marks)

**Suggested Readings:**

1. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
2. Findley's Practical Physical Chemistry, B.P. Lavitt, Longman.
3. Practical Physical Chemistry, S.R. Palit and S.K. De, Science.
4. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
5. Experiments in Physical Chemistry, D.P. Shoemaker
6. Experiments in Physical Chemistry, D.V. Jahagirdhar.
7. Senior Practical Physical Chemistry by B.D. Khosla, V. Garg and A. Gulati.
8. Advanced Practical Physical Chemistry, J.B. Yadav, Goel Publishing House.

**M.Sc- Chemistry**  
**Semester-I**

**CHE-109 Practical – III**  
**Organic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Qualitative Analysis (20 Marks)  
Separation, purification and identification of compounds of binary mixtures by chemical tests, derivatization. (One set to be given in the examination)
1. Organic Synthesis (20 Marks)
  - (i) p-nitroacetanilide from aniline
  - (ii) anthranilic acid from phthalic anhydride
  - (iii) 2,4-dinitrophenylhydrazine from chlorobenzene
  - (iv) P-aminophenol from nitrobenzene
2. Viva-Voce (05 marks)
3. Note-Book (05 marks)

**Suggested Readings:**

1. A Hand book of Organic Analysis -Qualitative and Quantitative by H.T. Clarke, and revised by B.Haynee, Edward Arnold, London 1975.
2. Vogel's Text Book of Practical Organic Chemistry by B.S. Furhen et. al., Longman-Group Ltd.
3. Systematic Qualitative Organic Analysis by H. Middleton, Edward Arnold (Publishers) Limited, London 1959.
4. Elementary Practical Organic Chemistry by Arthur I. Vogel, EX CBS Publishers and Distriibutors.
5. Experiments in Organic Chemistry by Louis, F. Fieser, D.C. Heath and Company Boston, 1955.

## M.Sc- Chemistry

### Semester-II

#### CHE-201: Inorganic Chemistry-II (Organometallic Chemistry & Molecular Clusters)

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

#### Unit –I

Valence electron count (16/18 electron rules), Total electron count (TEC), Compliance and violation of the 18 electron rule, Metal Carbonyls – Structure, bonding and infrared spectroscopy of metal carbonyls, bonding modes of CO, symmetry of metal carbonyls; synthesis-and reactivity of metal carbonyls; substituted metal carbonyls and related compounds; Synthesis, bonding, structure and important reactions of transition metal nitrosyl, dinitrogen complexes and tertiary phosphine and N-Heterocyclic carbenes as ligand in organometallic compounds, synthesis and important reactions of carbonyl hydrides.

#### Unit-II

Types of M-C bonds: Alkenes and Alkynes as ligands-synthesis, bonding and important reactions of metal bound alkenes and alkynes, concept of Umpolung; Complexes with M-C double and triple bonds-synthesis, bonding and important reactions of carbenes and carbynes; Synthesis and reactivity of  $\sigma$  bonded metal-alkyls and  $\eta^1$ -aryl compounds; Synthesis, structure and properties of complexes with cyclic and acyclic polyenyl  $\pi$  bonded ligands, metallocenes and bent metallocenes, allyl groups as ligands, Davis-Green- Mingos (DGM) rules;  $^1\text{H}$ NMR and  $^{13}\text{C}$  Spectra of organometallic compounds.

#### Unit-III

Characteristic reactions of organometallic complexes: Substitution, oxidative addition, reductive elimination, Migratory insertion, Catalytic Hydrogenation of alkenes, Hydrocyanation, Hydrosilylation, Hydroformylation, Methanol Carbonylation and Olefin Oxidation- Monsanto process, Cativa and Wacker process, Olefin- Metathesis, C-C and C-N cross coupling reactions, Olefin polymerization, Metallocene based and Post-metallocene based catalysts, Oligomerisation reactions.

### Unit-IV

Halide clusters  $[\text{Re}_2\text{X}_8]^{2-}$ ,  $\text{Re}_3\text{X}_9$  and Carboxylate clusters-  $\text{Re}_2(\text{RCOO})_4\text{X}_2$ ,  $\text{Mo}_2(\text{RCOO})_4$ ; Low nuclearity metal carbonyl clusters, High nuclearity carbonyl clusters, capping rule, Mingo's rule, Carbide clusters, Isolobal analogy; Main Group Clusters- Structure and bonding in the closo, nido, arachno – boranes and carboranes, styx notation; Wade-Mingos and Jemmis electron counting rule; Clusters having interstitial main group elements, cubane clusters and naked or Zintl clusters; Isolobal relationships between main-group and transition metal fragments.

#### Suggested Readings:

1. Basic Organometallic Chemistry; Concepts, Synthesis and Applications B.D. Gupta and A.J. Elias; University Press (India), 2010.
2. Organometallic Chemistry; R.C. Mehrotra and A. Singh, New Age International.
3. The Organometallic Chemistry of the Transition Metals; R.H. Crabtree, John Wiley.
4. Introduction to Cluster Chemistry- D.M.P. Mingos and J. Wales, Prentice Hall, 1990
5. Molecular Clusters: A Bridge to solid-state Chemistry, T.P. Fehlner, J.F. Halet and J-Y. Saillard, Cambridge University press, 2007.
6. Chemistry of Elements, 2nd Edition, N.N. Greenwood and E.A. Earnshaw, Butterworth-Heinemann, 1997.
7. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
8. Inorganic Chemistry: Principles of structure and reactivity, J.E. Huhey, E.A. Keiter and R.L. Keiter, Pearson Education, 2006.
9. R. West, Solid State Chemistry and its Applications, John Wiley & Sons, 1984.



**M.Sc- Chemistry**  
**Semester-II**

**CHE-202: Physical Chemistry-II**  
**(Physical Chemistry: Concepts & Applications)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit -I**

Thermodynamics and Phase Equilibria: Third law of thermodynamics (Nernst heat theorem, determination of absolute entropy and its limitation); Concept of phase, The Gibb's phase rule, derivation of the phase rule, Clausius Clapeyron equation and its applications; Phase diagram for one component system, (H<sub>2</sub>O, CO<sub>2</sub> and Sulphur system); Phase diagram for two completely miscible components systems, Eutectic systems, Calculation of eutectic point, systems forming solid compounds A<sub>x</sub>B<sub>y</sub> with congruent and incongruent melting points.

**Unit-II**

Chemical Dynamics: Kinetics of reaction in solution, Debye smoluchowski reaction; Influence of pressure, ionic strength, solvent on reaction rates; salt effect; Kinetics of catalytic reactions : acid base catalysis, enzyme catalysis (Michaelis - Menton treatment, evaluation of Michaelis's constant for enzyme - substrate binding by Lineweaver - Burk plot) Competitive and noncompetitive inhibition, Heterogeneous catalysis.

**Unit-III**

Statistical Thermodynamics: Concept of distribution, thermodynamic probability and most probable distribution, Types of statistics: Maxwell Boltzmann, Bose-Einstein & Fermi dirac statistics and its statistical thermodynamic formulation, Idea of microstates and macrostates, Thermodynamic probability for three types of statistics and most probable distribution states for them; Concept of partition function, its physical significance, molar and atomic partition function and their relation various thermodynamic properties; Lagrange's undetermined multiplier, Stirling's approximation,

**Unit-IV**

Quantum Mechanics: Angular momentum operators in Cartesian coordinates, eigen function & eigen values, commutation relation between angular momentum operators ( $L_x, L_y, L_z, L^2$ ) commutation relation between components of total orbital angular momentum and ladder operators, commutator of [ $L^2, L_+$ ] and [ $L^2, L_-$ ], application of ladder operators to an eigen function of  $L_z$ ; Schrodinger wave equation for Rigid rotator, energy of rigid rotator, space quantization; Schrodinger wave equation for linear harmonic oscillator and its solution using factorization method, zero point energy;

**Suggested Readings:**

1. Thermodynamics for Chemists, Affiliated East -West Press.
2. Thermodynamics, I.M. Klotz and R.M. Rosenbers, Benzamin.
3. An Introduction to Chemical Thermodynamics, R.P. Rastogi and R.R. Misra, Vikas Pub.
4. Chemical Kinetics, K.J. Laidler, McGraw Hill.
5. Kinetics and Mechanism, A. A. Frost and R.G. Pearson, John Wiley and Sons.
6. Chemical Kinetics and Reaction Dynamics, Springer, 2006.
7. Elements of Statistical Thermodynamics, 2nd edition, Addison Wesley (1974)
8. Physical Chemistry, G.W. Castellan, Narosa.
9. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
10. Quantum Chemistry, I.M. Levine, Prentice Hall.
11. Quantum Chemistry, B. K. Sen, Kalyani Publishers
12. Quantum Chemistry, R. Prasad, New Age International.

**M.Sc- Chemistry**  
**Semester-II**

**CHE-203: Organic Chemistry-II**  
**(Organic Reaction Mechanism)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit –I**

Aromatic Electrophilic Substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams. The ortho/para ratio, ipso attack, orientation in other ring systems. Quantitative treatment of reactivity in substrates and electrophiles. Diazonium coupling, Vilsmeier reaction, Gattermann-Koch reaction. Vilsmeier-Haack reaction, Reimer-Tiemann reaction, Bischler-Napieralski reaction, Pechmann reaction, Houben-Hoesch reaction, Fries rearrangement

Aromatic Nucleophilic Substitution: The  $ArS_N1$ ,  $ArS_N2$ , Benzyne and  $S_{RN}1$  mechanisms. Reactivity – effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements. General aspects of generation, structure, stability and reactivity of arynes.

**Unit -II**

Elimination Reactions: The E2, E1 and E1cB mechanisms. Orientation Effects in Elimination Reactions, Reactivity – effects of substrate structures, attacking base, the leaving group and the medium. Saytzeff and Hoffman rules, Stereochemistry of E2 elimination reactions and eclipsing effects in E2 eliminations. Dehydration of alcohols, Elimination not involving C-H bonds. Mechanism and orientation in pyrolytic elimination.

Addition to Carbon-Carbon Multiple Bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, regio- and chemoselectivity, orientation and reactivity. Addition to cyclopropanation.

Hydrogenation of double and triple bonds, hydrogenation of aromatic rings. Hydroboration. Michael reaction. Sharpless asymmetric epoxidation.

**Unit -III**

Addition to Carbon-Hetero Multiple Bonds: Hydration and Addition of Alcohols to Aldehydes, Ketones and Acids. Addition -Elimination Reactions of Ketones and Aldehydes, Reactivity of carbonyl compounds towards addition. Addition of Grignard reagents, organozinc and organolithium reagents to carbonyl and  $\alpha,\beta$ -unsaturated carbonyl compounds, Wittig reaction.

Mechanism of metal hydride reduction of saturated and unsaturated carbonyl compounds, acids, esters and nitriles.

Mechanism of condensation reactions involving enolates – Aldol, Knoevenagel, Claisen, Mannich, Robinson Mannich, Reformatsky, Benzoin, Perkin and Stobbe reactions. Hydrolysis of esters and amides, ammonolysis of esters.

#### Unit -IV

Rearrangements: Classification and general mechanistic treatment of nucleophilic, free radical and electrophilic rearrangement, Dienone-Phenol; Benzil-benzilic acid; Favorskii; Wolff; Homologation of aldehyde and ketones by diazomethane; Neber; Curtius; Lossen; Schmidt reaction; Meisenheimer; Bayer-Villiger; Steven; Wittig; Benzidine rearrangements; Chapman; Wallach.

#### Suggested Readings:

1. A Guide Book to Mechanism in Organic Chemistry, Peter Sykes, Longman
2. Organic Chemistry, R. T. Morrison and R. N. Boyd, Prentice Hall of India.
3. Advanced Organic Chemistry, J. March, 3rd Edn. McGraw Hill, 1991.
4. Organic Chemistry, J. Clayden, N. Greeves, S. Warren, and P. Wothers, Chapter 30, Oxford University Press, Oxford
5. Organic Chemistry, L. G. Wade, Pearson Education
6. Organic Chemistry, G. Solomons and C. Fryhle, John Wiley & Sons (Asia) Pte Ltd.
7. Organic Chemistry, J. McMurry, Asian Books Pvt. Ltd.
8. Organic Chemistry, S.H. Pine, 5th Edn., McGraw Hill, 1987.
9. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Trinity.

**M.Sc- Chemistry**  
**Semester-II**

**CHE-204****Supramolecular & Photochemistry**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Introduction of Supramolecular chemistry, Nature of binding interactions in Supramolecular structures: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and van der Waals interaction. Molecular and chiral recognition- Self-Organization, Self-Assembly and Preorganization, lock and key analogy, Covalent self-assembly based on preorganization - inclusion complexes, host-guest chemistry, Utilisation of H-bonds to create Supramolecular structures, Use of H-bonds in crystal engineering and molecular recognition, Chelate and macrocyclic effects.

**Unit-II**

Binding of cationic, anionic, ion pair and neutral guest molecules

Synthesis and structure of crown ethers, coronads, cryptands, spherands, calixarenes, cyclodextrins, cyclophanes, cryptophanes, carcerands, hemicarcerands, metallomacrocycles, catenanes, rotaxanes and helicates

Industrial Applications of Supramolecular Systems and Supramolecular catalysis

**Unit-III**

Principles and concepts: An overview of: Laws of photochemistry, Beer-Lambert law, electronic energy levels, atomic and molecular term symbols, singlet-triplet state, intensity and strength of electronic transition, selection rules for electronic transition, Jablonski diagram, Franck-Condon, breakdown of selection rules and Photo-physical processes: De-excitation processes for the excited molecules (fluorescence, phosphorescence, delayed emission, non-radiative relaxation)

**Unit-IV**

Photophysical kinetics of unimolecular processes, quantum yield expressions, photophysical kinetics of bimolecular processes, excimer and exciplex, kinetics of luminescence quenching: static and dynamic, Stern-Volmer analysis, deviation from Stern-Volmer kinetics. Photoinduced electron transfer rates, free energy dependence of electron transfer on rate, Photoinduced energy transfer, Fluorescence Resonance Energy Transfer FRET.

**Suggested Readings:**

1. Supramolecular Chemistry: Concepts & Perspectives, J. M. Lehn, Wiley-VCH (1995).
2. Perspectives in Supramolecular Chemistry, Vol. 2: Crystal Engineering and Molecular Recognition, G. R. Desiraju, Wiley: Chichester (1995).
3. Supramolecular Chemistry: A Concise Introduction, J. L. Atwood and J.W. Steed, John Wiley & Sons (2000).
4. Supramolecular Chemistry, F. Vogtle, John Wiley, (1991).
5. Crystal Engineering. The Design of Organic Solids, G.R. Desiraju, Elsevier, (1989).
6. Introduction to Supramolecular Chemistry, Helena Dodzuick, Springer, (2002).
7. Fundamentals of Photochemistry, K.K. Rohatagi-Mukherjee, Wiley Eastern, (1978).
8. Essentials of Molecular Photochemistry, Von A. Gilbert and J. Baggott, Blackwell Scientific Publication, Oxford (1991).
9. Molecular Photochemistry, N.J. Turro, W.A. Benjamin, (1965).
10. Introductory Photochemistry, A. Cox and T. Camp, McGraw Hill, (1971).

**M.Sc- Chemistry**  
**Semester-II**

**CHE-205****Group Theory & Molecular Spectroscopy**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Symmetry Elements and Operations, Pure Rotations ( $C_n$  Rotations), Improper Rotations, Rotation-Reflection ( $S_n$ ) & Rotation-Inversion ( $\bar{n}$ ) Axes.

Point Groups: Low Symmetry Point Groups ( $C_1$ ,  $C_i$ ,  $C_s$ ), Simple Axial Point groups ( $S_n$ ,  $C_{nv}$ ,  $C_{nh}$ ), Dihedral Groups ( $D_n$ ,  $D_{nd}$ ,  $D_{nh}$ ), Platonic Solids & the "Cubic" Groups ( $T_d$ ,  $O_h$ ,  $I_h$ ), The "Infinite Groups" ( $C_{\infty v}$  and  $D_{\infty h}$ ), Points Groups & Chirality, Point Groups & Dipole Moment. Multiplication Tables (i.e., operation 1 followed by operation 2) for point groups.

**Unit-II**

Similarity Transforms, Classes of Symmetry Elements. Naming Representations (Mulliken Symbols), Subgroups and Non Commutative Operations.

Representations of Groups, Irreducible Representations, Character Tables. Their derivations and use of their contents. Matrix Representation of Symmetry Operations. The "Full Form" of the Character Table.

Application of group theory to atomic orbitals in ligand fields, molecular orbitals, hybridization.

**Unit-III**

Rotational spectroscopy of diatomic molecules based on rigid rotator approximation. Determination of bond lengths and atomic masses from microwave data, intensities of rotational spectral lines, isotopic effect, non-rigid rotator, spectra of polyatomic linear molecules and symmetric top molecules, First order Stark effect.

The vibrating diatomic molecule, force constant, zero point energy, simple harmonic vibrator, anharmonicity, Morse potential, overtones, hot bands, diatomic vibrating rotators, P,Q,R branches, vibration of polyatomic molecules, normal mode of vibrations, Breakdown of the Born-Oppenheimer approximation, Nuclear spin effect.

Pure rotational Raman spectra of linear molecules, vibrational Raman spectra, mutual exclusion principle, polarization of the light and Raman effect, depolarization of Raman lines. Symmetry of normal modes, Use of Group Theory in assignment of spectra and selection rules for IR & Raman transitions.

Electron Spectroscopy- Diatomic molecules. Selection rules. Breakdown of selection rules. Franck-Condon factors.

**Suggested Readings:**

1. Theory of Groups and its applications to Physical Problems, S. Bhagavantam, and T. Venkatarayudu, Academic Press, New York, (1969).
2. Symmetry in molecules, J.M., Hollas, Chapman & Hall, (1972).
3. Group theory and Chemistry, David M. Bishop, Dover Publications (1989).
4. Chemical Applications of Group Theory, F. A. Cotton, 3<sup>rd</sup> Edition, John Wiley (1990).
5. Molecular Symmetry and Spectroscopy, P.R. Bunker, and P. Jensen, NRC Press, Ottawa, Canada, (1998).
6. Symmetry in Chemistry, H.H. Jaffe and M. Orchin, Dover Publications (2002).
7. Introduction to Molecular Spectroscopy, G.M. Barrow, McGraw Hill (1962).
8. Basic Principles of Spectroscopy, R.Chang, McGraw Hill, (1971).
9. Physical Methods for Chemists, R.S. Drago, Saunders College, (1992).
10. Fundamentals of Molecular Spectroscopy, C.N. Banwell, , 4<sup>th</sup> Edition, Tata McGraw Hill, (1994).
11. Modern Spectroscopy J.M. Hollas, 4<sup>th</sup> Edition, John Wiley (2004).



**M.Sc- Chemistry**  
**Semester-II**

**CHE-207**  
**Communication Skills**

Maximum Marks: 50  
Theory Examination: 40  
Internal Assessment: 10 Max. Time: 2 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Human Communication (Theoretical perspective): Its uniqueness, its nature, models of communication. Types of Human communication, Language, non-verbal communication, logic and reasoning, lateral thinking. The concept of facilitating: factors, barriers and filters in communication; the seven C's of effective communication, Preparing for interviews, CV/Biodata.

**Unit -II**

Self communication, interpersonal communication, dyadic communication , small group communication. Public communication . Mass Communication, Reliability of communication.  
Input and Evaluation Processes (Practice): Listening (process, comprehension, evaluation). Reading (process, comprehension, evaluation). Watching (process, comprehension, evaluation). Email Do's and Don'ts.

**Unit -III**

Output and Interaction Processes (Practice): Speech (conversation, interview, group discussion, public speech). Writing (spontaneous writing, guided writing, creative writing). Organizing ideas (noting, summary, flow charts, concept maps). Correspondence (personal, business).

**Unit-IV**

Science / Scientific Writing (Theory and practice): Goals and Objectives. Ethics in writing. Structure of documents. Language and grammar. Illustrations and aids. Writing proposals and instructions. Making presentations. Formatting documents. Drafts and revisions. Editing. Writing popular science / journal article.

**Suggested Readings:**

1. Communicating a social and career focus, K. M. Berko, Andrew D. Wolvyn and Darlyn R. Wolvyn, Houghton Mifflin Co., Boston (1977)
2. The Craft of Scientific Writing (3rd Edition), Michael Alley, Springer, New York (1996)
3. Science and Technical Writing – A Manual of Style (2nd Edition), Philip Reubens (General editor), Routledge, New York (2001)
4. Writing Remedies – Practical Exercises for Technical Writing Edmond H. Weiss, Universities Press (India) Ltd., Hyderabad (2000)
5. Effective Technical Communication, M. Ashraf Rizvi, Tata Mc Graw – Hill Publishing Co. Ltd., New Delhi (2005)

## SEMESTER – II

### Organic Chemistry of Polymers

DCEC

(4Hrs /week) Credits: 4

#### Unit I

Classification of polymers by properties (morphological, elastomeric, thermoplastic, thermoset, emulsion polymers, suspension polymers), and structures (aliphatic hydrocarbons, aromatic hydrocarbons, polysaccharides, polyesters, polyamides, polyurethanes, polyphosphazenes, silicones, glasses, phenol-formaldehyde resins)

#### Unit 2

Applications of polymers (elastomeric, adhesives, membranes, agricultural mulch films. Introduction to polymer structures. Synthesis of different classes of polymers (condensation polymers, free radical polymers, coordination polymers). Mechanisms of polymerizations by anionic, cationic, free radical and coordination catalysis.

#### Unit 3

Synthesis of polymers by radical, emulsion, suspension, and ionic mechanisms, Copolymers, Functionalization of synthetic (hydrocarbons) and natural polymers (cellulose, lignin) by use of chemical reactions, Crosslinking of polymers, Stereochemistry of polymers, cis trans rubbers, poly(methylmethacrylate) polymers.

#### Unit 4

Natural Polymers (cellulose, starch, lignin, galactomannans, xanthan gum, alginic acid). Biodegradable Polymers, with special reference to Polyvinyl alcohol, polylactic acid, and cellulose esters. Applications of biodegradable polymers.

#### Books suggested:

1. Principles of Polymerization, George Odian, 4th. Edition, Wiley-Interscience (2004).
2. Textbook of Polymer Science, Fred W. Billmeyer, 3rd. Ed., John Wiley and Sons (Asia) (2013).
3. A Textbook of Polymer Chemistry, M.S.Bhatnagar, S.Chand & Co., (New Delhi) (2014 reprint).
4. Biodegradable Polymers for Industrial Applications, Ray Smith, Ed., CRC Press (New York, Woodhead Publishing Co., (Cambridge) (2005).

*K. D. Swamy*

*Chaitanya*

**M.Sc- Chemistry**  
**Semester-II**

**CHE-208 Practical- I**  
**Inorganic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Determination of some metal ions, such as iron, nickel, manganese, chromium, vanadium etc. and fluoride, nitrite and phosphate etc. by Spectrophotometric Method. (20 Marks)
2. Quantitative Analysis:  
Separation and determination of two metal ions such as Ag- Cu, Cu- Ni, Cu- Zn, Ni- Zn, Cu-Fe etc. involving volumetric and gravimetric methods. (20 Marks)
3. Viva-Voce (05 Marks)
4. Note Book (05 Marks)

**Suggested Readings:**

1. A Text Book of Macro and Semi-micro Quantitative Analysis, A.I.Vogel, Orient Longman.
2. A Vogel's Text Book of Quantitative Inorganic Analysis, J. Bassett, R.C. Denney, G.B. Jaffery and J. Menaham, Longman, London.
3. Laboratory manual: Analytical Chemistry - principles and techniques by Larry G. Hargis, Prentice Hall.

**M.Sc- Chemistry**  
**Semester-II**

**CHE-209: Practical-II**  
**Physical Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Chemical Kinetics

- (i) Study kinetics of hydrolysis of an ester in the presence of acid.
- (ii) Saponification of ethyl acetate.
- (iii) Compare the relative strength of acids

2. Potentiometry

- (i) Determine the strength of strong acid by potentiometric titration with strong base.
- (ii) Determine the strength of weak acid by potentiometric titration with strong base.
- (iii) Determine the strength of a given solution of ferrous ammonium sulphate by potentiometric titration with  $K_2Cr_2O_7$  solution.

3. pH metry

- (i) Determine the strength of strong acid by pH-metric titration with strong base.
- (ii) Determine the strength of weak acid by pH-metric titration with strong base.

4. Refractometry

- (i) Determine the refractive index of the given liquid.

\*Two Experiments 2x20 = 40 marks

5. Viva-Voce

(05 Marks)

6. Note-Book

(05 Marks)

**Suggested Readings:**

1. Practical Physical Chemistry, A.M. James and F.E. Prichard, Longman.
2. Findley's Practical Physical Chemistry, B.P. Lavitt, Longman.
3. Practical Physical Chemistry, S.R. Palit and S.K. De, Science.
4. Experimental Physical Chemistry, R.C. Das and B. Behera, Tata McGraw Hill.
5. Experiments in Physical Chemistry, D.P. Shoemaker
6. Experiments in Physical Chemistry, D.V. Jahagirdhar.
7. Senior Practical Physical Chemistry by B.D. Khosla, V. Garg and A. Gulati.
8. Advanced Practical Physical Chemistry, J.B. Yadav, Goel Publishing.

**M.Sc- Chemistry**  
**Semester-II**

**CHE-210 Practical- III**  
**Organic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Isolation of natural products (20 Marks)
  - (i) Isolation of caffeine from tea leaves
  - (ii) Isolation of piperine from black pepper
  - (iii) Isolation of  $\beta$ -carotene from carrots
  - (iv) Isolation of lycopene from tomatoes
  - (v) Isolation of limonene from lemon peel
  - (vi) Isolation of eugenol from cloves
  
2. Organic Synthesis (20 Marks)
  - (i) p-bromoaniline from acetanilide
  - (ii) benzoic acid from benzoin
  - (iii) caprolactone from cyclohexanone
  - (iv) tribromobenzene from aniline
  
3. Viva-Voce (05 Marks)
4. Note-Book (05 marks)

**Suggested Readings:**

1. Vogel's Text Book of Practical Organic Chemistry by B.S. Furhen et. al., Longman-Group Ltd.
2. Elementary Practical Organic Chemistry by Arthur I. Vogel, EX CBS Publishers and Distributors.
3. Experiments in Organic Chemistry by Louis, F. Fieser, D.C. Heath and Company Boston, 1955.
4. Practical Organic Chemistry by Mann and Saunders.
5. Organic chemistry experiments: Microscales and semimicroscales, Campbell, B.N. and Ali M, McCarty M, Brooks/Cole, 1994.
6. Techniques and experiments for organic chemistry, Ault A., University Science Books, 1998.
7. Multiscale operational organic chemistry: A problem solving approach to laboratory course, Lehman, Prentice Hall, 2002.
8. A Hand book of Organic Analysis -Qualitative and Quantitative by H.T. Clarke, and revised by B.Haynee, Edward Arnold, London 1975.

**M.Sc- Chemistry**  
**Semester-III**

**CHE 301: Organic Spectroscopy**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Ultraviolet and Visible Spectroscopy: Various electronic transitions (185 -800 nm), Beer-Lambert law, effect of solvent on electronic transitions, ultraviolet bands for carbonyl compounds, unsaturated carbonyl compounds, dienes, conjugated polyenes. Fieser-Woodward rules for conjugated dienes and carbonyl compounds, ultraviolet spectra of aromatic and heterocyclic compounds. Steric effect in biphenyls.

Infrared Spectroscopy: Instrumentation and sample handling. Characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines. Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds). Effect of hydrogen bonding and solvent effect on vibrational frequencies, overtones, combination bands and Fermi resonance. FT IR, IR of gaseous, solids and polymeric materials.

**Unit-II**

Nuclear Magnetic Resonance Spectroscopy: General introduction and definition, chemical shift, spin-spin interaction, shielding mechanism, mechanism of measurement, chemical shift values and correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides & mercapto), complex spin-spin interaction between two, three, four and five nuclei (first order spectra), spin system-Pople notation, virtual coupling. Stereochemistry, concept of topicity, effect of enantiomeric and diastereomeric protons, hindered rotation, Karplus curve -variation of coupling constant with dihedral angle. Fourier transform technique, Resonance of other nuclei -F, P. Further tools for simplification (chemical and instrumental) to elucidate structures by NMR - Deuteration, changing solvents, trifluoroacetylation, basification and acidification, shift reagents, spin decoupling.

### Unit-III

Mass Spectrometry: Introduction, ion product ion - EI, CI, FD and FAB, factors affecting fragmentation, ion analysis, ion abundance. Mass spectral fragmentation of organic compounds, common functional groups, molecular ion peak, metastable peak, Nitrogen rule, molecular weight determination molecular formula from isotopic ratio data, isotope profile of halogen compounds, factors affecting reaction pathways, fragmentation pattern - simple cleavage, retro-Diels Alder, Hydrogen transfer rearrangement like scrambling, ortho effect, McLafferty rearrangement, fragmentation patterns of hydrocarbons, alcohols, phenols, ethers, aldehydes, ketones, esters, carboxylic acids, amines, nitro, amides, nitriles.

Carbon-13 NMR Spectroscopy: General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyl carbon), coupling constants. Nuclear Overhauser effect (NOE).

### Unit-IV

Problems

Problems pertaining to sections A, B and C.

#### Readings:

1. Introduction to Spectroscopy- A Guide for Students of Organic Chemistry, 2ndEdn. By Donald L. Pavia, Gary M. Lampman and George S. Kriz .Saunders Golden Sunburst Series. Harcourt Brace College Publishers, New York.
2. Spectrometric Identification of Organic Compounds, R. M. Silverstein, G. C.Bassler and T. C. Morrill, John Wiley.
3. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hall.
4. Spectroscopic Methods in Organic Chemistry, D. H. Williams and I. Fleming, Tata McGraw-Hill.
5. Spectroscopy of Organic Compounds by P.S. Kalsi, Wiley Estern, New Delhi.
6. Organic Spectroscopy by William Kemp, John Wiley.
7. Organic Mass Spectrometry by K.G. Das & E.P. James, Oxford & IBH Publishing Co.
8. Organic Spectroscopy (Principles & Applications) by Jagmohan.



**M.Sc- Chemistry**  
**Semester-III**

**CHE 302: Inorganic Spectroscopy**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Vibrational Spectroscopy: Spectra and symmetry, Selection rules, Symmetry and shapes of AB<sub>2</sub>, AB<sub>3</sub>, AB<sub>4</sub>, AB<sub>5</sub> and AB<sub>6</sub>, modes of bonding of ambidentate ligands, ethylenediamine and diketonate complexes, changes in spectra of donor molecules on coordination, change in symmetry on coordination, bond strength frequency shift relations, Use of symmetry to determine the number of active infrared and Raman lines, Application of resonance Raman Spectroscopy particularly for the study of active sites of metalloproteins as myoglobin and haemoglobin.

**Unit-II**

Nuclear magnetic resonance spectroscopy : Application of chemical shifts, signal intensities and spin-spin coupling to structure determination of inorganic compounds carrying NMR active nuclei like <sup>1</sup>H, <sup>11</sup>B, <sup>15</sup>N, <sup>19</sup>F, <sup>29</sup>Bi, <sup>31</sup>P, <sup>183</sup>W, <sup>195</sup>Pt, etc. Effect of fast chemical reactions, coupling to quadrupolar nuclei, NMR of paramagnetic substances in solution, nuclear and electron relaxation time, the expectation value of  $\langle S_z \rangle$ , contact shift, pseudo contact shift, factoring contact and pseudo contact shift for transition metal ions. Contact shift and spin density,  $\pi$  delocalization, simplified M.O. diagram for Co(II) and Ni(II), Application to planar tetrahedral equilibrium, Contrast agents.

**Unit-III**

Nuclear Quadrupolar Resonance (NQR) Spectroscopy: Quadrupolar moment, energy levels of a quadrupolar nucleus and effect of asymmetry parameters and energy levels. Effect of an external magnetic field, selected examples for elucidation of structural aspects of inorganic compounds using NQR spectroscopy.

Electronic paramagnetic resonance spectroscopy: Basic Principle and EPR spectrometers, Presentation of spectra, Hyperfine coupling, Hyperfine splitting in isotropic systems, Factors affecting magnitude of g, EPR of triplet states, zero field splitting, Kramer's rule, survey of EPR spectra of first row transition metal ion complexes, applications to inorganic free radicals, study of electron exchange reactions.

## Unit-IV

Mossbauer Spectroscopy: Basic Principles, Spectral display, Doppler shift and recoil energy, isomer shift and its interpretation, quadrupole interactions, effect of magnetic field on Mossbauer spectra, applications to metal complexes, metal carbonyls, Fe-S cluster and tin compounds, etc. Partial quadruple splitting and geometry of the complexes.

Presentation and interpretation of mass spectrum, effect of isotopes on appearance of mass spectrum, Applications of mass spectroscopy to inorganic compounds - finger print application, molecular weight determination, evaluation of heat of sublimation of high melting solids.

### Suggested Readings:

1. John Roboz, Introduction to Mass Spectrometry: Instrumentation and Techniques, Interscience (1968).
2. D.C. Harris and M.D. Bertolucchi, Symmetry and Spectroscopy: An introduction to vibrational and electronic spectroscopy, Dover Publications (1990).
3. N.B. Colthup, L.H. Daly and S.E. Wiberley, Introduction to Infrared and Raman Spectroscopy, 3<sup>rd</sup> Ed .Academic Press (1990).
4. E.A.O. Ebsworth, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publications (1991).
5. L. Que Jr., Physical Methods in Bioinorganic Chemistry, University Science Books (2000).
6. F. Hammer, Inorganic Spectroscopy and related topics, Sarup & Sons Publications (2008).
7. R. S. Drago, Physical Methods in Inorganic Chemistry, East-West Press Pvt. Ltd. New Delhi (2012).
8. E.I. Solomon and A.B.P. Lever, Inorganic Electronic structure and Spectroscopy, Wiley (2013).
9. C.N. Banwell and E. M. McCash, Fundamentals of Molecular spectroscopy, Tata McGraw HillPub. Co. New delhi (2016)

**M.Sc- Chemistry**  
**Semester-III**

**CHE 303: Analytical Chemistry**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Error analysis: Methods of sampling and associated errors, Classification of errors, Propagation of errors, treatment of errors, Normal distribution, Tests of Significance and Confidence Limits.

Chromatography: Types. Ion exchange chromatography, planar chromatography - paper and Thin Layer Chromatography, Stationary and mobile phases, Gas chromatography – Theory, instrumentation and applications. Liquid-liquid partition chromatography, High Performance Liquid Chromatography (HPLC), Reverse phase chromatography.

**Unit-II**

Atomic Absorption Spectroscopy: Principle, instrumentation, resonance line, its natural width, Doppler effect, broadening due to pressure, Hollow cathode lamp, Application to alkali and alkaline earth metals, sensitivity and detection limits, interferences in AAS and their elimination.

Flame photometry: Theory of flame photometry, flame temperature, Emission Flame photometry intensity of spectral lines, selection of optimum working conditions, application of flame photometry in trace metal analysis.

**Unit-III**

Thermal Methods: Introduction to Thermogravimetric Analysis (TGA) and Derivative Thermogravimetric Analysis (DTG), static thermogravimetry and dynamic thermogravimetry, Instrumentation, thermogram, factors affecting thermograms, application of thermogravimetry. Reaction kinetics – Kinetics by single and multiple heating rates, Differential Thermal Analysis (DTA), DTA theories, DTA curves, factors affecting DTA curves, Instrumentation, applications of DTA, simultaneous determination in thermal analysis, Correlation of DTA and TGA data with examples.

Differential Scanning Calorimetry (DSC) Introduction, Instrumentation, Power compensated DSC, Heat Flux DSC, DSC curves, factors affecting DSC curves, applications.

### Unit-IV

Electrogravimetry: Current-voltage relationship during an electrolysis, decomposition potential, constant current electrolysis, constant cathode potential electrolysis, apparatus, electrodes, mercury cathode, applications physical properties of electrolytic precipitates , chemical factors of importance in electrodeposition, Electrolytical methods without cathode potential control; Coulometric analysis : Coulometric methods of constant electrode potential and coulometric titrations- Apparatus and applications; Amperometric titrations , anodic stripping voltammetry, and cyclic voltammetry

#### Suggested Readings:

1. D.A. Skoog, D. M. West, F. J. Holler, S.R. Crouch, Fundamentals of Analytical Chemistry, 8th Edition, Thomson (2004).
2. A.I. Vogel, A text book of Quantitative Analysis, 5th Edition Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, ELBS (1989).
3. A. K. De, S. M. Khopkar and R. A. Chalmers, Solvent Extraction of Metals, Van Nostrand, Reinhold (1970).
4. L. R. Snyder and J. J. Kirkland, Introduction to Modern Liquid Chromatography, 2nd Edition, Wiley (1979).
5. Jose A. C. Broekaert, Analytical Atomic Spectrometry with flames and Plasmas, Wiley-VCH (2002).
6. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley &

**M.Sc- Chemistry**  
**Semester-III**

**CHE 304(a): Nuclear and Radiation Chemistry**  
**(Inorganic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Nuclear structure and nuclear stability, Mass and binding energy, Nuclear Models: Liquid drop model, Shell model, Fermi gas model, collective model, optical model, concept of spin, parity electric and magnetic moments.

**Unit-II**

Modes of Decay:  $\alpha$  decay,  $\beta$  decay, electron captures,  $\gamma$  de-excitation, internal conversion, artificial radioactivity; Nuclear reactions: Energetic, cross-section, centre of mass system, angular momentum, mechanism of nuclear reaction by compound nucleus model, statistical model, nuclear fission and fusion, nuclear reactors, Heavy ion induced reactions, Accelerators and cyclotron.

**Unit-III**

Elements of Radiation Chemistry: Interaction of radiation with matter (photoelectric effect, Compton effect and pair production) radiation dosimetry, radiolysis of water and some aqueous solutions.

Applications of radioactivity: Probing by isotopes, preparation of radioisotopes, Szilard-Chamers' reaction, Concept of tracers, chemical yield, radiochemical purity, Application of radiotracers in Chemical Sciences, uses of nuclear radiations.

**Unit-IV**

Nuclear Methods: Activation Analysis – Neutron Activation Analysis (NAA) NAA - Principle, Application and Limitation, Isotope Dilution Analysis (IDA) - Principle, Application and Limitation, Radiometric titrations.

Detection of Nuclear Radiation: Gas filled counters – Ionization chamber; Proportional counter and G.M. counters. Scintillation detectors; Solid state detectors

**Suggested Readings:**

1. G. Friedlander, J. W. Kennedy, E.S. Macias and J. M. Miller, Nuclear and Radiochemistry, John Wiley & Sons (1981)
2. R. D. Evans, Atomic Nucleus (1955)
3. S. Glasstone, Source book of Atomic Energy (1969)
4. G. T. Seaborg, Man made elements (1963).
5. H. J. Arnikar, Essentials of Nuclear Chemistry (1982).
6. C. Keller, The Chemistry of Transuranium Elements (1971).
7. J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; Comprehensive Inorganic Chemistry, Vol. 5, Pergamon Press, Oxford (1973).
8. B. C. Harvey, Introduction to Nuclear Chemistry Prentice-Hall (1969).

**M.Sc- Chemistry**  
**Semester-III**

**CHE 305(a): Bio-Inorganic  
Chemistry**  
**(Inorganic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Metal Ions in Biological Systems: Fundamentals of inorganic biochemistry, essential, non-essential and trace elements in bio-systems,  
Role of alkali/alkaline earth metals in bio-systems; Bioinorganic chemistry of  $\text{Na}^+$ ,  $\text{K}^+$ ,  $\text{Mg}^{2+}$  and  $\text{Ca}^{2+}$ , Ionophores, active transport of cations across membranes, sodium pump, Calcium pump, Calcium carriers, Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter.

**Unit-II**

Role of metal ions in replication and transcription process of nucleic acids; metal ions in nucleotide systems, effect of metal ions on nucleic acids, Metal complexes of polynucleotides, nucleosides and nucleic acids (DNA & RNA), Template temperature, stability of DNA.  
Role of metal ions in oxygen carriers and synthetic oxygen carriers: Porphyrins, metalloporphyrins, Hemoproteins, structure and functions of hemoglobin and myoglobin, synthetic oxygen carrier model systems

**Unit-III**

Fixation of dinitrogen biologically and abiologically, biotransformation of non-metallic inorganic compounds, Nitrogenase, model for nitrogenase, metal- $\text{N}_2$  complexes, photosynthesis and chlorophyll.  
Metal Storage Transport and Bio-mineralization- Ferritin, transferrin, and siderophores.  
Metal ions as antioxidants, metal ion enhancing catalytic activity of enzymes (Biocatalysts). Inhibitions as competitive and non-competitive.

**Unit-IV**

Metallo-protein and enzymes: Zinc Enzymes – Carboxypeptidase, Carbonic anhydrase, alkaline phosphatase and alcohol dehydrogenase, Iron Enzymes – Catalase, Peroxidase and Cytochrome P- 450, Copper Enzymes – Superoxide dismutase, blue copper electron transfer enzyme, Molybdenum oxatransferase enzymes – Xanthine oxidase  
Coenzymes – Vitamin  $\text{B}_{12}$  and Vitamin  $\text{B}_6$

**Suggested Readings:**

1. S.J. Lippard and J.M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, 1994.
2. I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, Bioinorganic Chemistry, University Science Books, Mill Valley, 1994
3. S. J. Lippard, Progress in Inorganic Chemistry, Wiley-Interscience, 1991.
4. M.N. Huges, The inorganic Chemistry of Biological Processes; John Wiley and Sons.
5. N.N.Greenwood and A. Earnshaw, Chemistry of the Elements, Pergamon, 1985.
6. James A.Cowan, Inorganic Biochemistry, VCH Publishers, 1993.



**M.Sc- Chemistry**  
**Semester-III**

**CHE-307 Practical- I**  
**(Inorganic Chemistry Specialization)**

Max. Marks: 50  
Time: 6 hrs.

1. Synthesis of inorganic complexes/compounds, their characterization and interpretation by various physicochemical methods, viz. IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other from the existed literature.
  - (i) Metal acetylacetonates- eg.  $\text{VO}(\text{acac})_2$ ,  $\text{Mn}(\text{acac})_3$ ,  $\text{Cr}(\text{acac})_3$ . *Inorg. Synth.* 1957, 5, 130; 1963, 1, 183.
  - (ii) Preparation of Ferrocene, *J. Chem. Educ.* 1966, 43, 73; 1976, 53, 730.
  - (iii) Preparation of triphenyl phosphine  $\text{Ph}_3\text{P}$ , and its transition metal complexes.
  - (iv)  $[\text{Co}(\text{NH}_3)_5\text{Cl}]\text{Cl}_2$ ;  $[\text{Co}(\text{NH}_3)_5\text{NO}_2]\text{Cl}_2$ ;  $[\text{Co}(\text{NH}_3)_5\text{ONO}]\text{Cl}_2$
  - (v) Reaction of Cr(III) with multidentate ligands, a kinetics experiment. *J. Am. Chem. Soc.*, 1953, 75, 5670.
  - (vi)  $\text{Ni}(\text{dmg})_2$ ,  $[\text{Ni}(\text{en})_3]\text{S}_2\text{O}_3$ ,  $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$
  - (vii) Metal complexes of dimethyl sulfoxide (IR):  $\text{CuCl}_2 \cdot 2\text{DMSO}$ ,  $\text{RuCl}_2 \cdot 4\text{DMSO}$  *J. Chem. Educ.*, 1982, 59, 57.
  - (viii) Synthesis and thermal analysis of group II metal oxalate hydrates.
  - (ix) Preparation of copper glycine complex-cis and trans bis (glycinato Cu( II); *J. Chem. Soc. Dalton* 1979, 1901; *J. Chem Edu.* 1982,59, 1052.
  - (x) Other new novel synthesis reported in literature from time to time
  
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**Suggested Readings:**

1. Synthesis and Characterisation of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. Inorganic Preparations: a systematic course of preparations by Alexander King, London, T. Murphy

**M.Sc- Chemistry**  
**Semester-III**

**CHE-308 Practical- II**  
**(Inorganic Chemistry Specialization)**

Max. Marks: 50  
Time: 6 hrs.

1. Estimation and Separation Processes
  - (i) Separation of cations and Anions by Column Chromatography- Ion exchange
  - (ii) Paper and Thin Layer Chromatography: For Identification of metal cations and complexes.
  - (iii) Solvent Extractions - Metal ion separation. Effect of pH, solvent, time.
  - (iv) Identification of Inorganic compounds using spectroscopic methods (IR, UV, NMR, Mass, TGA & DTA ).
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**Suggested Readings:**

1. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. Inorganic Preparations: a systematic course of preparations by Alexander King, London, T. Murphy

**M.Sc- Chemistry**  
**Semester-III**

**CHE-309 Practical- III**  
**(Inorganic Chemistry Specialization)**

Max. Marks: 50  
Time: 6 hrs.

1. Instrumentation

- (i) Estimation of metal ions by Atomic Absorption Spectrophotometry.
- (ii) Determination of pK value of an indicator Spectrophotometrically.
- (iii) Conductometrically – Composition of mixture of weak and strong acids, precipitation and displacement titrations.
- (iv) pH – metry – Composition of mixture of strong and weak acids, pKa value of organic acids.
- (v) Determination of stoichiometry of zirconium-alizarin Red-S complex : Mole-ratio method.
- (vi) Determination of stoichiometry and stability constant of Fe-thiocynate, Fe-Phenanthroline/copper-ethylenediamine complex by Slope-ratio method.
- (vii) Determination of concentration of sulphate ions in the given solution by Turbidimetry.

- 2. Viva-Voce (05 Marks)
- 3. Note Book (05 Marks)

**Suggested Readings:**

- 1. Vogel's Textbook of Quantitative Analysis, revised J. Bassett, R. C. Denney, G.H. Jeffery and J.Mendham, ELBS.
- 2. Laboratory manual: Analytical Chemistry - principles and techniques by Larry G. Hargis, Prentice Hall.

**M.Sc- Chemistry**  
**Semester-III**

**CHE 304(b): Advanced Quantum Chemistry**  
**(Physical Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Chemical Bonding: Valence bond method, valence bond method to hydrogen, hydrogen molecule ion (their symmetric and anti symmetric solution without actual valuation of various integrals, energy of molecular hydrogen system, LCAO-MO approximation, Concept of resonance and its role in the stability of hydrogen molecule ion..

**Unit-II**

Schrodinger wave equation for hydrogen atom, separation of variable in polar spherical coordinates and its solution, Principle, azimuthal and magnetic quantum numbers and the magnitude of their values, probability distribution function, radial distribution function and shape of atomic orbitals (s, p & d).

**Unit-III**

Variation Method: Quantum mechanical treatment of Helium atom and the failure of rigorous quantum mechanical method, need of approximate methods, Approximate Methods: The variation theorem, Linear variation Principle, perturbation theory (first order, second order and non degenerate), Applications of variation method and perturbation theory to the Helium atom. Self-Consistent-Field theory.

**Unit-IV**

Molecular Orbital Theory: Huckel molecular orbital (HMO) theory of linear and cyclic conjugated systems, Applications of HMO theory (i) Set up and solve Huckel determinant equation (ii) Calculate resonance energy (iii) Wave functions for molecular orbitals (iv) Molecular diagrams of (a) Ethylene molecule (b) Butadiene (c) Cyclobutadiene (d) Cyclopropenyl system (cyclopropenyl radical and the related ions).

**Suggested Readings:**

1. Physical Chemistry, G.W. Castellan, Narosa
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, I.M. Levine, Prentice Hall.
4. Quantum Chemistry, B. K. Sen, Kalyani Publishers
5. Quantum Chemistry, R. Prasad, New Age International.
6. Quantum Chemistry & Spectroscopy – Thomas Engel
7. Quantum Chemistry MC. Quarrie D.A. Viva
8. Physical Chemistry A molecular approach Univ. Science (2001)

**M.Sc- Chemistry**  
**Semester-III**

**CHE 305(b): Advanced Electrochemistry**  
(Physical Chemistry Specialization)

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Chemical Electrodics: Rate of charge- transfer reactions under zero field, under the influence of an electric field, the equilibrium exchange current density, the non equilibrium drift-current density (Butler-Volmer) equation. Some general and special cases of Butler-Volmer equation, the high-field and low-field approximations, physical meaning of the symmetry factor ( $\beta$ ), a preliminary to a second theory of  $\beta$ , a simple picture of the symmetry factor and its dependence on overpotential. Polarizable and non-polarizable interfaces.

**Unit-II**

Advanced Electrochemistry: Overpotential, Exchange current density, Butler-Volmer equation, Polarizable and non-polarizable interfaces. Tafel equations. Electrochemical Processes: Difference between kinetically and mass transport controlled electrochemical processes. Difference between single step and multiple step electrode reactions.

**Unit-III**

Corrosion: Forms of Corrosion, Uniform corrosion, galvanic corrosion, pitting corrosion, crevice corrosion, intergranular corrosion, stress corrosion cracking, corrosion Dfatigue, fretting corrosion, dealloying, hydrogen embrittlement, erosion corrosion, microbial induced corrosion, filliform corrosion and exfoliation. Fundamental of electrolytic corrosion: theories and kinetics, corrosion prevention. Batteries, fuel cells and electro catalysis.

**Unit-IV**

Applications of Electrochemistry: Brief introduction and applications of various electrochemical methods: Principle of electrochemical methods such as chronoamperometry, cyclic voltammetry, chronopotentiometry, coulometry, ac-impedance spectroelectrochemistry and hydrodynamic methods . Electrochemical electricity generators (fuel cells), brief idea about H<sub>2</sub>- O<sub>2</sub>, hydrocarbon - air, and natural gas & CO -air fuel cells. Electricity storage: some important quantities in electricity storage (energy density, power density), desirable conditions for an ideal energy storage device , storage of electricity using the lead-Acid battery, dry cell, silver-zinc cell and Sodium- Sulfur cell.

**Suggested Readings:**

1. Electrochemistry, S. Glasstone, Affiliated East -West Press
2. Physical Chemistry, G.W. Castellan, Narosa.
3. Electrochemical Methods : Fundamentals and applications, 2nd Ed., A.J. Bard and L. R. Faulkner  
John Wiley & Sons : New York, 2002.
4. Modern Electrochemistry 1 : Ionics 2nd Ed., Springer (1998), J.O. M. Bockris & A.K. Reddy.
5. Modern Electrochemistry 2B: Electrode in Chemistry, Engineering, Biology and Environmental  
Science 2nd Ed., Springer (2001), J.O. M. Bockris & A.K. Reddy.
6. Modern Electrochemistry 2A: Fundamentals of Electrode 2nd Ed., Springer (2001), J. O. M.  
Bockris, A. K. N. Reddy and M. E. Gamboa- Aldeco.
7. Crow, D.R. Principles and Applications of Electrochemistry, 4th Edition Chapman and Hall,  
London 1994.

**M.Sc- Chemistry**  
**Semester-III**

**CHE-307 Practical- I**  
**(Physical Chemistry Specialization)**

Max. Marks: 50  
Time: 6 hrs.

**1. Conductometry**

- (i) Determine the strength of acetic acid by titrating it against ammonium hydroxide
- (ii)  $\text{Ba}(\text{NO}_3)_2$  vs.  $\text{Na}_2\text{SO}_4$  titration
- (iii)  $(\text{HCl} + \text{CH}_3\text{COOH} + \text{CuSO}_4)$  mixture vs.  $\text{NaOH}$

**2. Potentiometry**

- (i)  $\text{AgNO}_3$  vs.  $\text{KCl}$  titration
- (ii) Determination of dissociation constant of weak acid ( $\text{H}_3\text{PO}_4$ ).

**3. Ultrasonic Interferometry**

- (i) Determination of speed of sound for various liquids.

**4. Flame Photometry**

- (i) To determine the concentration of  $\text{Na}^+$ ,  $\text{Li}^+$ ,  $\text{Ca}^{++}$  ions in the given solution

Two Experiments  $2 \times 20 = 40$  Marks

**5. Viva – Voce = 05 Marks**

**6. Notebook = 05 Marks**

**M.Sc- Chemistry**  
**Semester-III**

**CHE-308 Practical- II**  
**(Physical Chemistry Specialization)**

Max. Marks: 50  
Time: 6 hrs.

**1. pHmetry**

- (i)  $\text{H}_3\text{PO}_4$  vs. NaOH
- (ii) HCl vs.  $\text{NH}_4\text{OH}$
- (iii)  $\text{CH}_3\text{COOH}$  vs.  $\text{NH}_4\text{OH}$
- (iv) Determine the dissociation constant of weak acid.

**2. Refractometer**

- (i) To determine percentage composition of liquids in the given binary mixture.

**3. Colorimeter**

- (i) Verify Lambert Beer's Law and
- (ii) Determine the concentration of  $\text{KMnO}_4/\text{K}_2\text{Cr}_2\text{O}_7$  in a solution of unknown concentration colorimetrically.

**4. Polarography**

- (i) Determination of half wave potential of  $\text{Pb}^{2+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Co}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Ni}^{2+}$ .

Two Experiments  $2 \times 20 = 40$  Marks

5. Viva – Voce = 05 Marks

6. Notebook = 05 Marks



**M.Sc- Chemistry**  
**Semester-III**

**CHE-309 Practical- III**  
**(Physical Chemistry Specialization)**

Max. Marks: 50  
Time: 6 hrs.

**1. Dipolemetry**

- (i) To determine the dipole moment of a liquid

**2. Polarimetry**

- (i) Determination of specific rotation for optically active substance
- (ii) Estimation of concentration of optical active substance in the given solution.
- (iii) Determination of rate constant for hydrolysis/inversion of sugar

**3. Thermochemistry**

- (i) Determination of heat of neutralization
  - (a) NaOH vs. HCl
  - (b) NaOH vs. CH<sub>3</sub>COOH

**4. Chemical Kinetics**

- (i) To determine the temperature coefficient for the I<sup>st</sup> order reaction.

Two Experiments 2\*20 = 40 Marks

5. Viva – Voce = 05 Marks

6. Notebook = 05 Marks

**M.Sc- Chemistry**  
**Semester-III**

**CHE 304(c): Concerted Reactions and Greener Modes of Organic Synthesis**  
**(Organic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Concerted Reactions-I: Molecular orbital symmetry, frontier orbital of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system classification of pericyclic reactions, Woodward-Hoffmann correlation diagram. FMO & PMO approach. Electrocyclic reaction - conrotatory and disrotatory motions.  $4n$ ,  $4n+2$ , allyl systems, Ring opening of cyclopropyl halides and tosylates. Cycloaddition-antarafacial and suprafacial additions,  $4n$ ,  $4n+2$  systems,  $2+2$  addition of ketenes, isocyanates, 1,3-dipolar cycloaddition and cheletropic reactions.

**Unit-II**

Concerted Reaction-II: Cycloadditions-antarafacial and suprafacial additions,  $4n$  and  $4n+2$  systems,  $2+2$  addition of ketenes, isocyanates, 1,3-dipolar cycloadditions and Cheletropic Reactions. Sigmatropic Rearrangements, suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties, retention and inversion of configuration, [3,3] and [5,5] sigmatropic rearrangements, detailed treatment of Sommelet-Hauser, Claisen and Cope rearrangements. Introduction to ene reactions.

**Unit-III**

Green Chemistry-I: Principle of Green chemistry and its applications: Basic Principle and need of green chemistry, Different tools for green synthesis (Elementary idea of green reagent, green solvent, green catalyst, solid phase, greener source of energy) atom economy, Role of biocatalysts in green synthesis – enzyme catalyzed oxidation, reduction and hydrolytic reactions, synthesis involving basic principle of green chemistry-synthesis of adipic acid and BHC synthesis of Ibuprofen. Principles of ultrasound and microwave assisted organic synthesis. Reactions in ionic liquids.

**Unit-IV**

Green Chemistry-II: Photochemistry of carbonyl compounds (Norrish type I and type II changes, photoreaction of cyclic ketones, Paterno-Buchi reaction and Photoreduction. Photochemistry of olefins and 1,6-Butadiene (cis-trans isomerisation, dimerisation and cycloadditions). Chemistry of vision. Di- $\pi$ -methane rearrangement, enone and dienone rearrangements, photochemistry of aromatic compounds (substitution, isomerization, cyclization and cycloaddition reactions), Photo-Fries rearrangement, photolysis of nitrile esters and Barton reaction, Hoffman-Loeffler-Freytag reaction.

**Suggested Readings:**

1. Organic Chemistry, Morrison and Boyd.
2. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.
3. Pericyclic reactions, Mukherji S.M., Mcmillan.
4. Orbital interaction in chemistry, Albright T., Burdee J and Whango M, Wiley VCH.
5. Frontier Orbitals and Organic Chemical Reactions, I. Fleming, Wiley, London, 1976.
6. Pericyclic Reactions- A text Book, S. Sankararaman, Wiley VCH, 2005.
7. Modern Molecular Photochemistry by N. J. Turro.
8. Organic Photochemistry by J. M. Coxan and B. Halton.
9. Essentials of Molecular Photochemistry by A. Gilbert and J. Baggot.
10. Organic Photochemistry and Photobiology, CRC Handbook, Edited by W. M. Horspool and P. S. Song.
11. Fundamentals of Photochemistry, K.K. Rohtagi & Mukherjee, Wiley Eastern.
12. Photochemistry, J.G. Calvert and J.N. Pitts, Wiley.
13. Photochemistry and Spectroscopy, J.P. Simons, Wiley Interscience.
14. Principles and Applications of Photochemistry by Brian Wardle.

**M.Sc- Chemistry**  
**Semester-III**

**CHE 305(c): Reagents for Organic Synthesis**  
**(Organic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Organometallic reagents (Main group elements) Preparation, properties and applications of following reagents in organic synthesis with mechanistic details.

Organolithium, Organomagnesium, lithium cuprates, organocadmium, organozinc, higher organoboranes, organosulphur reagents, organosilicon reagent, organoiodines (III).

**Unit-II**

Organometallic reagents (Transition metals): Organo titanium (Tebbe olefination) Organo chromium compounds Organo iron, Organo nickel, Organo cobalt, Organo Palladium complexes, Metal mediated C-C and C-X coupling reactions: Heck, Stille, Suzuki, Negishi and Sonogashira, Nozaki-Hiyama, Buchwald-Hartwig, Ullmann coupling reactions, directed ortho metalation. Organo ruthenium reagents (Grubbs 1st and 2nd generation catalyst).

**Unit-III**

Reduction: Introduction, reduction of alkenes, alkynes, aromatic hydrocarbons, alcohols, aldehydes, ketones, carboxylic acid and their derivatives, nitriles, nitro, nitroso, azo and oxime groups with mechanistic details highlighting chemo and stereoselective aspects.

**Unit-IV**

Oxidation: Introduction, Oxidative processes, Hydrocarbons: alkenes (to epoxide, Sharpless asymmetric epoxidation, Jacobson and Shi epoxidation, to diols (cis and trans), to carbonyl compounds with and without bond cleavage) aromatic rings, saturated C-H groups (activated and unactivated), aldehydes, ketones, ketals, carboxylic acids, amines, hydrazines, sulfides. Oxidation with ruthenium tetroxide and thallium (III) nitrate.

**Suggested Readings:**

1. F. A. Cary and R. I. Sundberg, *Advanced Organic Chemistry, Part A and B*, 5th Edition, Springer, 2009.
2. W. Carruthers, *Modern Methods of Organic Synthesis*, Cambridge University Press, 1996.
3. *Advanced Organic Chemistry Reactions, Mechanisms & Structures*, J. March, Wiley.
4. S. Warren, *Organic Synthesis, The disconnection Approach*, John Wiley & Sons, 2004.
5. J. Tsuji, *Palladium Reagents and Catalysts, New Perspectives for the 21st Century*, John Wiley & Sons, 2003.
6. I. Ojima, *Catalytic Asymmetric Synthesis*, 2nd edition, Wiley-VCH, New York, 2000.
7. W. Carruthers, *Modern Methods of Organic Synthesis*, Cambridge University Press, 1996.
8. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, 2001.
9. R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons, 1994.
10. L. Kuerti and B. Czako, *Strategic Applications of named Reactions in Organic Synthesis*, Elsevier Academic Press, 2005.
11. *Designing Organic Synthesis*, S. Warren, Wiley.
12. *Modern Synthetic Reactions*, H.O. House, W.A. Benzamin.
13. Solomons, T. W. G., *Organic Chemistry* 6th ed, 1996.
14. *Protecting group in Organic synthesis*, Greene T, Wuts P.G.M., John Wiley & Sons, 1989.
15. E. J. Corey and X-M. Cheng, *The logic of chemical synthesis*, John-Wiley & Sons, New York, 1989.
16. K. C. Nicolaou, *Classics in Total Synthesis of Natural Products*, Vol. I (1996) & Vol. II (2003).
17. *Strategic applications of named reactions in organic synthesis*, Kurti L. and Czako B., Academic Press, 2005.

**M.Sc - Chemistry**  
**Semester-III**

**CHE-307 Practical- I**  
**Organic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Separation and identification of organic mixtures of polyfunctional compounds containing two (solid-solid, solid-liquid, liquid-liquid) components by chemical tests and checking purity of individual components using TLC. IR, NMR spectra to be used for functional group identification.
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**CHE-308 Practical- II**  
**Organic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Spectrophotometric (UV-vis ) Estimations :
  - (i) Amino acids
  - (ii) Proteins
  - (iii) Carbohydrates
  - (iv) Ascorbic acid
  - (v) Aspirin
  - (vi) Caffeine
  - (vii) Cholesterol
2. Studies of TLC, column chromatography and paper chromatography for organic mixtures.
3. Viva-Voce (05 Marks)
4. Note Book (05 Marks)

**CHE-309 Practical- III**  
**Organic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. **Multi-step synthesis:**
  - (i) Benzanilide from benzene
  - (ii) Benzophenone – benzopinacole – benzopinacolone
  - (iii) Benzoin – benzil – benzilic acid
  - (iv) cyclohexanone – cyclohexanone oxime - caprolactone
  - (v) p-nitrobenzanilide from Benzophenone

Or

any other suitable multistep synthesis
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 405: Computational Chemistry**

Maximum Marks: 100  
Theory Examination: 60  
Internal Assessment: 40  
Max. Time: 4 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Introduction to Operating system (UNIX, Windows) and programming language. Algorithm, Flow charts. Writing simple programs, converting a flow chart into a program. Using graphics package plotting (a)  $y = x$ ,  $x^2$ ,  $\sin(x)$ ,  $\tan(x)$  (b) wave functions for s, p, and d – orbitals.

**Unit-II**

Numerical Methods: Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion. Numerical differentiation and integration. Statistical treatment of data, variance and correlations, linear regression, Curve fitting.

**Unit-III**

Using ChemDraw. Writing programs for van der Waals equation, pH titration, kinetics, radioactive decay, evaluation of lattice energy and ionic radii from experimental data. Elementary structural features such as bond lengths, bond angles, dihedral angles et c. of molecules extracted from a database such as Cambridge database.

**Unit-IV**

A brief outline of molecular mechanics, semi-empirical approximations, ab initio methods, basis sets and Z-matrix; Application of these computational methods for prediction of structural and electronic properties of molecules by using standard programs; FMOs in organic chemistry, crystal and ligand field calculations, computation of potential energy surfaces. Conformational analysis by molecular mechanics; Dynamical and structural studies of molecules using molecular dynamics simulations; Monte Carlo simulations of molecules.

**Suggested Readings:**

1. Introduction to Computer Science, P.K. Sinha
2. Let Us C, Yashwant Kanetker
3. Computational Chemistry, A.C. Norris.
4. Hunt, R.; Shelley, J. Computers and Common Sense, Prentice Hall.
5. Programming in Fortran 90 and 95, V. Rajaraman.
6. C. J. Cramer, Essentials of Computational Chemistry: Theories and Models, John Wiley & Sons, 2002.
7. D. Young, Computational Chemistry: A practical Guide for applying Techniques to Real World Problems, Wiley Interscience, 2001.
8. A. R. Leach, Molecular Modelling: Principles and Applications, Pearson Education, 2001.
9. J. B. Foresman, A. Frisch, Exploring Chemistry with Electronic Structure Methods. Gaussian Inc., 1996.
10. M. P. Allen and D. J. Tildesley, Computer Simulations of Liquids, Oxford, 1987
11. Organic Chemists book of Orbitals, by William L. Jorgensen and Lionel Salem; Wiley-VCH, 1973.
12. Killingbeck, J.P.; Hilger, Adam Microcomputer Quantum Mechanics.
13. Rajaraman, V.; RadhaKrishnan, V. An Introduction to Digital Computer Design, Prentice



**M.Sc- Chemistry**  
**Semester-IV**

**CHE 401(a): Chemistry of Main Group Elements**  
**(Inorganic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Stereochemistry and Bonding in Main Group Compounds: VSEPR Theory, Walsh diagrams (tri- atomic molecules), Hybridization including energetics of hybridization,  $d\pi-p\pi$  bonds, Bent rule and energetics of hybridization, Some simple substitution reactions of covalently bonded molecules of boron, silicon and nitrogen-(i) Atomic inversion (ii) Bery pseudo rotation (iii) Nucleophilic displacement (iv) Free radical mechanism.

**Unit-II**

Hydrogen, alkali and alkaline earth metals: Classification of hydrides - e-deficient, e-precise & e-rich hydrides, Application of crown ethers in extraction of alkali and alkaline earth metals.  
Noble gases: Isolation and properties. Preparation and structure of noble gas compounds  
Boron compounds: Preparation, structure, bonding, reactions and applications of boranes, carboranes, metalloboranes, metallocarboranes, boron halides, phosphine boranes, boron heterocycles, borazines.

**Unit-III**

Compounds of carbon and silicon: Fullerenes and their compounds, Intercalation compounds of graphite, Synthesis, structure, properties, and applications of carbon nano-tubes, Carbides, fluorocarbons, silanes, silicon halides, silicates, aluminosilicates and silicones.  
Syntheses and characterization of clays, pillared clays and zeolites, application of clays, pillared clays and zeolites with emphasis of catalyses

**Unit-IV**

Compounds of nitrogen group elements: Nitrogen activation. Oxidation states of nitrogen and their interconversion. Preparation, structure and bonding of PN compound, Oxyacids of Phosphorous, Phosphazenes.  
Compounds of oxygen group elements: Metal selenides, tellurides, oxoacids of Sulphur, Structural features and reactivity of SN heterocycles.  
Compounds of halogen group elements: Synthesis, properties, and applications of interhalogens, pseudohalogens, polyhalides, oxyacids and oxoanions of halogens

**Suggested readings:**

1. D.F. Shriver, P.W. Atkins and C.H. Langford, *Inorganic Chemistry*, Oxford Univ. Press, 1998
2. J.E. Huheey, E.A. Keiter and R.L. Keiter, *Inorganic Chemistry: Principle of Structure and Reactivity*, Pearson Education, 2004.
3. F.A. Carey, G. Wilkinson, C.A. Murillo and M. Bochman, *Advanced Inorganic Chemistry*, Wiley Interscience, 2003.
4. C.E. Housecroft and A.G. Sharpe, *Inorganic Chemistry*, Prentice Hall, 2005.
5. N.N Greenwood and A. Earnshaw, *Chemistry of the Elements*, Pergamon.
6. W.W. Porterfiels, *Inorganic Chemistry: A unified Approach*, Elsevier
7. A.G. Sharpe, *Inorganic Chemistry*, Pearson Education Ltd.
8. G. L. Miessler and D.A Tarr, *Inorganic Chemistry*, Pearson Publications.
9. G. Wulfsberg, *Inorganic Chemistry*, , University Science Books, Viva Book

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 402(a): Organotransition Metal Chemistry**  
**(Inorganic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Introduction and Classification of organometallic compounds by bond types viz. covalent, ionic, electron deficient and cluster compounds.

Alkyls and Aryls of Transition Metals: Types, routes of synthesis, stability and decomposition pathways, organocopper in organic synthesis.

**Unit-II**

Transition Metal  $\pi$ -Complexes: Transition metal  $\pi$ -complexes with unsaturated molecules- alkenes, alkynes, allyl, dienyl, arene and trienyl complexes, preparation, properties and nature of bonding and structural features. Important reactions related to nucleophilic and electrophilic attack on ligands and to organic synthesis.

**Unit-III**

Compounds of Transition Metal-Carbon Multiple Bonds: Alkylidenes, alkylidynes, low valent carbenes and carbynes- synthesis, nature of bond, structural characteristics, nucleophilic and electrophilic reactions on the ligands, role in organic synthesis

Transition Metal Compounds with Bonds to Hydrogen

**Unit-IV**

Organometallic Reagents: Principle, preparations, properties and applications of the reagents of metals/metalloids/ non-metals with mechanistic details: Li, Mg, B, Si, S, I, Ti, Cr, Fe, Co, Ni, Cu, Zn, Rh, Pd, Cd.

**Suggested readings:**

1. F. Basolo and R.G. Pearson, Mechanism of Inorganic Reactions; John Wiley and Sons, New York.
2. K.F. Purcell and J.C. Kotz ; Inorganic Chemistry; Holt-Sanders International Editions; Philadelphia.
3. J.P. Collman, L.S. Hegsdus, J .R. Norton and R.G. Finke, Principles and Application of Organotransition Metal Chemistry, University Science Books.
4. R.H. Crabtree, The Organometallic Chemistry of the Transition Metals; John Wiley.
5. R.C. Mehrotra and A. Singh, Organometallic Chemistry, New Age International.
6. Banerjea, Coordination Chemistry; Tata McGraw Hill.
7. B. Douglas, D.H. McDaniel and J.J. Alexander; Concepts and Models of Inorganic Chemistry; John Wiley and Sons Inc.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 403(a): Solid State  
Chemistry**

**(Inorganic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.**

**Unit-I**

Solid State Structure: Primitive lattice vectors - reciprocal lattice - crystal systems and desymmetrization schemes. Bravais lattices; closed packed structures, octahedral and tetrahedral holes, Crystal structures of some binary and ternary compounds such as fluorite, antiferite, rutile, antirutile, cristobalite, layer lattices-  $\text{CdI}_2$ ,  $\text{BiI}_3$ ,  $\text{ReO}_3$ ,  $\text{Mn}_2\text{O}_3$ , corundum, perovskite, Ilmenite and Calcite, Normal and inverse spinels.

**Unit-II**

Defects and Non-stoichiometry: Intrinsic and extrinsic defects- point defects, line and plane defects, vacancies- Schottky defects and Frenkel defects. Thermodynamics of Schottky and Frenkel defect formation, colour centres, non-stoichiometry and defects.

Metals, insulators and semiconductors, electronic structure of solids- band theory, band structure of metals, insulators and semiconductors. Intrinsic and extrinsic semiconductors, doping semiconductors, p-n junctions, superconductors, Optical and Magnetic properties.

Alloys- interstitial, substitutional and super conducting, Meissner effect, Hume -Rothery rules

**Unit-III**

Solid State Lasers (Ruby, YAG and tunable lasers): Inorganic phosphor materials; Synthesis and advantages of optical fibres over conducting fibres. Diffusion in solids, catalysis and Zone refining of metals.

Preparation of nanomaterials and their characteristic differences over bulk materials.

Principles of Electron Microscopy, Dynamic Light Scattering and characterization of nanomaterials.

**Unit-IV**

Symmetry elements in crystals, criteria for determining unit cell of lattice, stereographic projections, point groups ( illustration of R,  $\bar{R}$ , Rm, R/m,  $\bar{R}/m$  point groups only), Bragg condition, Miller indices for plane, space lattices, space groups P1,  $\bar{P}1$ , P2, P21, Pm, Pc, Cc, C2, Cm, C2/m.

Bragg method, Laue method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absences in diffraction pattern. Structure factor calculations for primitive, body-centered and face centered unit cells.

**Suggested readings:**

1. H.V. Keer, Principles of the Solid State, Wiley Eastern Ltd. New Delhi (1993).
2. A.R. West, Solid State Chemistry and its Applications, John Wiley & Sons New York (2005).
3. N. Hannay, Treatise on Solid State Chemistry, Plenum (1976).
4. A.K. Cheetham and P. Day, Solid State Chemistry Techniques, Clarendon Press, Oxford (1987)
5. G. Timp, Nanotechnology Springer-Verlag , New York. (1999).
6. N.N. Greenwood, Ionic crystals, lattice defects and non-stoichiometry,.
7. Material Science and Engineering. An Introduction, W.D. Callister, Wiley, New York (1985).
8. E. Moore and L. Smart, Solid State Chemistry: An Introduction 2<sup>nd</sup> Ed. Chapman & Hall (1996)
9. L. Smart, E.Moore, Solid State Chemistry (3<sup>rd</sup> Ed), Taylor & Francis (2005).
10. W. Massa, Crystal Structure Determination 2<sup>nd</sup> Ed. Springer (2004).
11. B.E. Warren, X-Ray Diffraction 1<sup>st</sup> Ed. Dover Publications (1990).
12. D. E. Sands, Introduction to Crystallography Reprint Dover Publications (1994).
13. M. Ladd and R. Palmer Structure Determination by X-ray Crystallography.
14. McKie and McKie,Essentials of Crystallography, Blackwell Scientific Publications, (1986).

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 404(a): Medicinal and Environmental Chemistry**  
**(Inorganic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Principles of Bioinorganic chemistry in Medicine, Evaluation of modern therapeutical agent , means of administering chemicals to humans, concentration effects, and dose-response relationship, Scope and developments of bioinorganic chemistry in medicine.

Biochemical basis of essential metal deficient diseases; Iron, copper and zinc deficiencies and their therapies;

Different classes of Inorganic drugs, Inorganic compounds as antacids, Drugs in hypo and hyper activity of thyroids, Inorganic drugs in dental carries, clinical disorders of alkali and alkaline earth metals and their remedies, lithium drugs in psychiatry.

**Unit-II**

Carcinogens and Carcinostatic agents, Role of zinc in tumour growth and inhibition, Anticancer activity and mechanism of platinum complexes, anticancer activity of Rhodium, copper and Gold complexes, anticancer activity of Selenium, alkylating agents as anticancer drugs, Thiosemicarbazones as anticancer drugs.

Antibacterial and antiviral properties of metal complexes and chelating drugs

Designing of chelating agents - Polyamino carboxylic acids and polyethylene amines as chelating drugs, chelating drug aspirin, chelating drugs where chelation and therapeutic activity are unrelated.

**Unit-III**

Fundamentals of Toxicity and their Detoxification, role of Selenium in Biological systems with reference to its essentiality and toxicity,

Mechanism of metal ion induced toxicity, interaction between orally administered drugs and metal ions in gut.

Ligand induced toxicity, interference with haemoglobin in oxygen transport system, interference with metallo-enzymes, beneficial effects of ligand chelation;

Nuclear medicine Therapy

### Unit-IV

Bio-distribution of the elements, Pollution and its Control a. Atmospheric pollution: gaseous air pollution, greenhouse effect and ozone shield, acid-rain particulate air pollution, radiation hazard. b. Aquatic pollution: agricultural and pesticidal inorganic and organic pollutants, marine pollution, oil spills and oil pollution. c. Industrial pollution: Thermal power, cement, fertilizer, sugar, distillery, drug, paper and pulp and nuclear industry pollution, mining and metallurgy, polymers, etc.

Environmental Toxicology and Detoxification Mechanism Chemical solutions to environmental problems, better biodegradability, kinetics of decomposition, clean technology.

#### Suggested readings:

1. S.J. Lippard and J.M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill Valley, 1994.
2. S. J. Lippard, Progress in Inorganic Chemistry, Wiley-Interscience, 1991.
3. Fenton, Biocoordination Chemistry, Oxford Chemistry Print, 1995.
4. Kaim and Schwederski, Bioinorganic: Inorganic Perspective in the Chemistry of Life, 1994.
5. S.E. Manahan, Environmental Chemistry; Lewis Publisher.
6. A.K. De, Environmental Chemistry; Wiley Eastern.
7. S.M. Khopkar, Environmental Pollution Analysis; Wiley Eastern.
8. S.K. Banerji, Environmental Chemistry; Prentice - Hall.



**M.Sc- Chemistry**  
**Semester-IV**

**CHE-406 Practical- IV**  
**Inorganic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Synthesis of inorganic complexes/compounds, their characterization and interpretation by various physicochemical methods, viz. IR, UV, Visible, NMR, magnetic susceptibility etc. Selection can be made from the following or any other from the existed literature.
  - (xi) Cis and trans isomers of  $[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$  *J. Chem. Soc.*, 1960, 4369.
  - (xii) Separation of optical isomers of  $\text{cis}[\text{Co}(\text{en})_2\text{Cl}_2]\text{Cl}$ , *J. Chem Soc.* 1960, 4369.
  - (xiii) Determination of Cr(III) complexes;  $[\text{Cr}(\text{H}_2\text{O})_6]\text{NO}_3 \cdot 3\text{H}_2\text{O}$ ;  $[\text{Cr}(\text{H}_2\text{O})_4\text{Cl}_2]\text{Cl} \cdot 2\text{H}_2\text{O}$ ;  $[\text{Cr}(\text{en})_3]\text{Cl}_3$ .
  - (xiv) Prussian blue
  - (xv)  $\text{Hg}[\text{Co}(\text{SCN})_4]$
  - (xvi)  $\text{K}_3[\text{Fe}(\text{C}_2\text{O}_4)_3]$ ,  $\text{K}_3[\text{Al}(\text{C}_2\text{O}_4)_3]$
  - (xvii) Mixed valence dinuclear complex of Manganese (III,IV).
  - (xviii) Preparation of Tin (IV) Iodide and Tin( II) Iodide (*Inorganic synthesis* 1953, 4, 119).
  - (xix) Tris(Thiourea ) Copper(I) Sulphate. (Estimation of Cu- Iodometrically)
  - (xx) Other new novel synthesis reported in literature from time to time
  
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**Suggested Readings:**

1. Synthesis and Characterisation of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. Inorganic Preparations: a systematic course of preparations by Alexander King, London, T. Murphy

**M.Sc- Chemistry**  
**Semester-IV**

**CHE-407 Practical- V**  
**Inorganic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Estimation and Separation Processes
  - (v) Ion Exchange – Cation and Anion Exchange.
  - (vi) Complexometry – using EDTA and Sequestering agent. Masking and Demasking.
  - (vii) Column Chromatography
  - (viii) Polarography- Estimation of Half Wave Potential
  - (ix) Identification of Inorganic compounds using spectroscopic methods (IR, UV, NMR, Mass, TGA & DTA ).
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**Suggested Readings:**

1. Synthesis and Characterization of Inorganic Compounds, W. L. Jolly, Prentice Hall.
2. Inorganic Preparations: a systematic course of preparations by Alexander King, London, T. Murphy

**M.Sc- Chemistry**  
**Semester-IV**

**CHE-408 Practical- VI**  
**Inorganic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Instrumentation

- (viii) Determination of stoichiometry of Fe-Phenanthroline/copper-ethylenediamine complex by Job's method of continuous variations.
- (ix) Flame photometric determinations of - sodium and potassium when present together; lithium/calcium/barium/strontium; calcium and magnesium in tap water.
- (x) Determination of stability constant of a complex by pH metry
- (xi) Determination of metal ions in a mixture sample by AAS.
- (xii) Potentiometry- redox titrations, precipitations, simultaneous determination of Halide ions.
- (xiii) Ion – selective electrodes- F, Ca, Na, K etc.

2. Viva-Voce

(05 Marks)

3. Note Book

(05 Marks)

**Suggested Readings:**

- 1. Vogel's Textbook of Quantitative Analysis, revised J. Bassett, R. C. Denney, G.H. Jeffery and J.Mendham, ELBS.
- 2. Laboratory manual: Analytical Chemistry - principles and techniques by Larry G. Hargis, Prentice Hall.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 401(b): Material  
Chemistry**  
(Physical Chemistry Specialization)

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Solid state Chemistry: Crystal structure, crystal types, crystal defects. Electronic structure of solids– Band theory, Superconductivity, Theory of insulators, semiconductors and metals. Optical and magnetic properties, alloys, solid state reactions

**Unit-II**

Inorganic Materials: Metals, alloys, glass, anionic clays, zeolites, simple and complex oxide and non-oxide ceramic systems, crystal structure, properties, structure- property relationship, defect chemistry, synthesis and characterization. Porous, soft materials, inorganic-organic hybrid and nanostructured materials.

**Unit-III**

Liquids: Liquids as dense gases, liquids as disordered solids, some thermodynamics relations, internal pressure and its significance in liquids, equation of state, critical constants, Different types of intermolecular forces in liquids, Different potential functions for liquids, additivity of pair potential approximation.

**Unit-IV**

Characteristics of Ionic Liquids : The thermal dismantling of an ionic lattice, characteristics of ionic liquids, the fundamental problems in the study of pure liquid electrolytes, models of simple ionic liquids: lattice oriented models (the vacancy model, the hole model), quantification of the hole model, the Furth approach to the work of hole formation, distribution function for the sizes of the holes and the average size of a hole.

**Suggested Readings:**

1. Principles of solid state, Keer H.V., Wiley Eastern
2. Solid state chemistry, Chakrabarty D.K., New Wiley Eastern.
3. Solid state chemistry: An introduction, Moore E., and Smart L., Chapman Hall, 1996.
4. Crystallography made crystal clear: A guide for users of macromolecular models, Rhodes G., Elsevier, 2006.
5. X-ray diffraction, Warren B., Dover Publications.

**M.Sc- Chemistry  
Semester-IV**

**CHE 402(b): Statistical & Non-Equilibrium Thermodynamics  
(Physical Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Statistical Thermodynamics (I): Partition function and factorization of partition function, Translational partition function and calculation of absolute entropy of an ideal monoatomic gas – Sackur - Tetrode equation. Separation of internal partition functions for diatomic molecule, Rotational & vibrational energy and entropy due to internal degrees of freedom. Calculation of various thermodynamic properties. Partition function for polyatomic molecules.

**Unit-II**

Statistical Thermodynamics (II): Partition function and equilibrium constant, effect of nuclear spin, isomolecular reaction, isotopic exchange reactions. Einstein theory and Debye theory of heat capacities of monatomic solids. Ensemble averaging, postulates of ensemble averaging. Micro canonical, canonical and grand canonical ensembles.

**Unit-III**

Transport Phenomenon: Diffusion coefficients, Fick's first and second laws, various relationships (flux and viscosity), (diffusion coefficient and mean free path), (thermal conductivity and mean free path of a perfect gas), Einstein relation, Nernst-Einstein equation, Stokes-Einstein equation, Einstein Smoluchowski equation..

**Unit-IV**

Non -Equilibrium Thermodynamics – I: General theory of non-equilibrium processes, entropy production and entropy flow; thermodynamic criteria for non-equilibrium states, entropy production in heat flow, mass flow, electric current, chemical reactions, Saxen's relation, Onsager's reciprocal relation, thermoelectric effects, thermomechanical phenomena and thermocells.

**Suggested Readings:**

1. Non-Equilibrium Thermodynamics Katchalasky, A. & Curren, P.F.
2. Nonequilibrium Statistical Mechanics.
3. Introduction to Statistical Thermodynamics Zwanzig, R., H. Dole.
4. Theoretical Chemistry, S. Glasstone, Affiliated East-West Press.
5. Thermodynamics, Lewis and Randall.
6. Chemical Physics, J.C. Slater.
7. Non-equilibrium Thermodynamics, C. Kalidas
8. Thermodynamics & Introduction to Thermostatistics by Callen H B
9. Physical Chemistry by Levine Ira N., Tata McGraw Hill
10. Physical Chemistry by Atkins P.W and Paula J. De, W.H. Freeman
11. Thermodynamics for chemists by Glasstone S.
12. Principles of Equilibrium Thermodynamics by Denbigh K G
13. McQuarrie, D. A. *Statistical Mechanics*

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 403(b): Fast Kinetics & Surface Phenomenon**

**(Physical Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Chemical Dynamics: Theory of absolute reaction rates, potential energy surfaces, activation energies, London — Eyring – Polanyi method for the calculation of energy of activation. Theories of unimolecular reactions: R.R.K. and R.R.K.M. theories.

**Unit-II**

Fast Reactions: Steady state kinetics of chain reaction such as (pyrolysis of acetaldehyde composition of ethane), photochemical (H<sub>2</sub>-Cl<sub>2</sub>) reactions & oscillatory reactions (Belousov-Zhabotinsky reaction), Phenomenological theory of reaction rates, Diffusion limited rate constant, Slow reactions, Linear free energy relationships, Relaxation methods for fast reactions. general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis, and NMR method.

**Unit-III**

Surface Phenomenon: Surface tension, capillary action, pressure difference across curved surface (Laplace eqn), vapour pressure of droplets, (Kelvin eqn), Gibb's adsorption isotherm, estimation of surface area (BET eqn), surface films on liquids (electro kinetic phenomenon), catalytic activity at surfaces. Surface active agents, classification of surface active agents, micellisation, hydrophobic interactions, critical micellar concentration, factors affecting CMC of surfactants, counter ions binding to micelles, thermodynamics of micellization-phase separation & mass action models, solubilization, microemulsion, reverse micelles.

**Unit-IV**

Surface Chemistry and Catalysis: Gibbs adsorption equation, Langmuir adsorption isotherm and its kinetic derivation for non- dissociative and dissociative adsorption, BET adsorption isotherm, its kinetic derivation and applications. Temporary and permanent catalytic poisons, activation energy for surface reactions. Comparison of homogeneous and heterogeneous reaction rates.

**Suggested Readings:**

1. Micelles, Theoretical and Applied Aspects, V. Moroi, Plenum.
2. Chemical Kinetics, K.J. Laidler, McGraw Hill
3. Theories of Chemical Reaction Rates, K.J. Laidler, McGraw Hill.
4. Theory of Rate Processes, S. Glasstone, K.J. Laidler and H. Eyring, McGraw Hill.
5. Reaction Kinetics Oxford Press (1997), M. J. Pilling and P. W. Seakins.



**M.Sc- Chemistry**  
**Semester-IV**

**CHE 404(b): Chemistry of  
Polymers**

**(Physical Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.**

**Unit-I**

Macromolecules: Basics of Polymers and Polymerization, Kinetics of Polymerization: Mechanism and Kinetics of chain growth polymerization: free-radical, cationic, anionic and coordination polymerization. Mechanism and Kinetics of step-growth polymerization. Comparison between step-growth and chain polymerization.

**Unit-II**

Molecular mass of Polymers: Concept of number average and mass average molecular weights, Methods of determination of molecular weights (1) viscometry (2) osmometry (3) sedimentation (4) Light Scattering methods (5) GPC (Debye & Zimm Plot)

**Unit-III**

Thermodynamics of Polymer Solutions: Poly-dispersity, Molecular mass distribution curves. Liquid Crystal Polymer Average end - to - end distance, average radius of gyration of polymer chains, statistical distribution of end - to - end dimensions, freely jointed chain in three dimensions, influence of bond angle restrictions. Flory Huggins lattice theory, limitations of lattice models.

**Unit-IV**

Basic & Commercial Polymers: Conducting polymers: Band structure; mechanism of conduction; synthesis and characterization of polyacetylene, polythiophene, polyaniline, polyethylene. Biodegradable polymers: Types of degradable polymers, Chemical and biodegradation. Applications of degradable polymers. Dendrimers, Hyperbranched – star polymers and Plasticizers. Polymer composites. Glass transition temperature (T<sub>g</sub>), factors influencing the glass transition temperature, importance of glass transition temperature (T<sub>g</sub>) and molecular weight, brief discussion on crystallization in polymers, amorphous polymers.

**Suggested Readings:**

1. K.W. Kolasinski, Surface Science: Foundations of Catalysis and Nanoscience, Wiley, 2002.
2. G.A. Somorjai, Y. Li , Introduction to Surface Chemistry and Catalysis, Wiley, 2010.
3. Physical chemistry of surfaces by Arthur W. Adamson 1990.
4. The chemical physics of surfaces by Roy S. Morrison, S. Roy, 1990.
5. H.R. Allcock, F.W. Lampe and James Mark, Contemporary Polymer Chemistry, Prentice Hall, Inc. (1990).
6. M.P. Stevens, Polymer Chemistry: An Introduction (2nd Edition) Oxford University Press 91990).
7. F.W. Billmeyer, Jr., Textbook of Polymer Science (3rd Edition) Wiley-Inter Science (1984) paperback.
8. A. Ravve, Principles of Polymer Chemistry.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE-406 Practical- IV**  
**Physical Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

**1. Conductometry**

- (i) Determine the cell constant of the given conductivity cell at room temperature and study the equivalent conductance vs square root of concentration for strong and weak electrolyte.
- (ii) Determination of concentration of Salicylic acid by
  - (iii) Salt line method (b) Double alkali method
- (iv) Determination of solubility and solubility product of sparingly soluble salt
  - i. ( $\text{AgCl}$ ,  $\text{PbSO}_4$ )
- (v) Determination of degree of hydrolysis and hydrolysis constant of aniline hydrochloride in aqueous solution.
  - i. Chloride in aqueous solution.

**2. Potentiometry**

- (i)  $\text{NaOH}$  vs.  $\text{H}_3\text{PO}_4$  titration
- (ii) Determination of solubility and solubility product of sparingly soluble salts ( $\text{BaSO}_4$ ) and  $\text{AgCl}$ .
- (iii) Determination of degree of hydrolysis of aniline hydrochloride
- (iv) Determine the dissociation constant of weak acid.

**3. Dipolemetry**

- (i) To determine the dielectric constant of various liquids

**4. Ultrasonic Interferrometry**

- (i) To determine the heat capacity of liquids and their mixtures

**M.Sc- Chemistry**  
**Semester-IV**

**CHE-407 Practical- V**  
**Physical Chemistry Practical**

Max. Marks: 50

Time: 6 hrs.

**1. Thermochemistry**

- (i) Determination of Heat of solution and Heat of hydration of  $\text{BaCl}_2$  and  $\text{CuSO}_4$
- (ii) Construction of phenol-water phase diagram and determination of upper critical solution temperature.
- (iii) Construction of binary Eutectic phase diagram of naphthalene-biphenyl system and determination of Eutectic temperature and Eutectic composition.

**2. Polarimetry**

- (i) Determination of percentage composition of optical substances in the given binary mixture (Glucose + Fructose or Tartaric acid)

**3. Chemical Kinetics**

- (i) Determination of activation energy for the hydrolysis of ethyl acetate in presence of acid.
- (ii) Study of Iodination of acetone.

**4. Turbidimetry**

- (i) Determine the concentration of sulphate ions in the given solution.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE-408 Practical- VI**  
**Physical Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

**1. pH metry**

- (i) Determination of composition of Copper amine complex from  $\text{CuSO}_4$  vs.  $\text{NH}_4\text{OH}$ .
- (ii) Determination of dissociation constant of  $\text{CH}_3\text{COOH}$  in acetone by titrating it with  $\text{KOH}$ .
- (iii) Determination of degree of hydrolysis of aniline hydro chloride.
- (iv) Preparation of buffer solution of various pH and the determination of their pH values.

**2. Colorimeter**

- (i) Determine the dissociation constant of an indicator.
- (ii) Study of iron-iron and iron-salicylic acid complexes.
- (iii) Determination of the composition of various mixtures spectrophotometrically: (i) Potassium dichromate and potassium permanganate (ii) Crystal violet and aurine

**3. Refractometer**

- (i) Study the variation of refractive index with concentration for  $\text{KCl}$  solution and there after determine the unknown concentration of given  $\text{KCl}$  solution.
- (ii) Determine the refractive index of simple organic liquids like methyl acetate, ethyl acetate, methanol, ethanol, n-hexane, chloroform.

**Suggested Readings:**

1. Matthews, G. Peter *Experimental Physical Chemistry*, 1st edition, Oxford University Press, 1985.
2. Shoemaker, D.P.; Garland, C.W.; Nibler, J.W. *Experiments in Physical Chemistry*, 6th edition (International Edition) McGraw Hill Inc., 1996.
3. Khosla, B.D.; Garg, V.C. Gulati, A. *Senior Practical Physical Chemistry*, 11<sup>th</sup> edition, R. Chand and Co., 2002.
4. Levitt, B.P. *Findlay's Practical Physical Chemistry*, 9th edition, Longman Group Ltd., 1973.
5. Practical Chemistry, A.M. James and F.E. Pricherd, Longman.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 401(c): Bioorganic and Medicinal Chemistry**  
**(Organic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Enzymes: Introduction and historical prospective, chemical and biological catalysis, remarkable properties of enzymes like catalytic power, specificity and regulation. Nomenclature and classification, extraction and purification. Fischer's lock and key and Koshland's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labelling. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible inhibition.

Mechanism of Enzyme Action: Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion.

**Unit-II**

Coenzyme chemistry: Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological function of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, NAD<sup>+</sup>, NADP<sup>+</sup>, FMN, FAD. Mechanisms of reactions catalysed by the above cofactors.

Mechanism of reactions catalyzed by enzymes (comparing the usual mechanism to enzyme catalysed mechanism): hydrolysis of esters, amides, phosphoesters, etc. C-C and C=C bond formation, oxidation, reduction. Enzyme catalyzed carboxylation and decarboxylation.

**Unit-III**

Development of new drugs, procedures followed in drug design, concepts of lead compound and lead modification, concepts of prodrugs and soft drugs, structure-activity relationship (SAR), factors affecting bioactivity, resonance, inductive effect, isosterism, bio-isosterism, spatial considerations. Theories of drug activity: occupancy theory, rate theory, induced fit theory.

Quantitative structure activity relationship. History and development of QSAR. Concepts of drug receptors. Elementary treatment of drug receptors interactions. Physico-chemical parameters: lipophilicity, partition coefficient, electronic ionization constants, steric, Shelton and surface activity parameters and redox potentials. LD-50, ED-50 (Mathematical equations excluded)

## Unit-IV

Synthesis, General Mode of Action and Medicinal Uses of Important Drugs in the following Categories. Antipyretic analgesics (paracetamol, aspirin, mefenamic acid), Antineoplastic (Methotrexate, Fluorouracil, chlorambucil), antimalarials (chloroquine, pyrimethamine), antitubercular (Isoniazid, ethambutol), antihelminthic (albendazole, thiabendazole), and sulfa drugs (sulfanilamide, dapsone).

### Suggested Readings

1. H. Dugas, Bioorganic Chemistry. A Chemical approach to enzyme action, 2nd Edn., Springer-Verlag, 1989.
2. D. E. Metzler, Biochemistry-The Chemical Reactions of a Living Cell, Academic Press, 1977.
3. Bioorganic Chemistry Frontiers Vol.2, Ed. H. Dugas, Springer-Verlag, pp.1-252, 1990.
4. Principles of Biochemistry By Lehninger
5. Principles of Biochemistry By Voet and Voet
6. Burger, Medicinal Chemistry, Vol. I-III, (1995) Wiley Interscience Publications, New York.
7. W. O. Foye, Principles of Medicinal Chemistry, 3rd Edition (1989), Lea & Febiger/Varghese Publishing House, Bombay.
8. D. Lednicer and L. A. Mitscher, The Organic Chemistry of Drug Synthesis, (1977) Vol. III, Wiley Interscience.
9. A. Kar, Medicinal Chemistry, (1993) Wiley Eastern Ltd., New Delhi.
10. N. K. Terrett, Combinatorial Chemistry, (1998) Oxford Univ. Press, Oxford.
11. Daniel Lednicer Strategies for organic drug synthesis and design (2009), John Wiley & Sons, New York.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 402(c): Heterocyclic Chemistry and Disconnection Approach**  
**(Organic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Replacement and Systematic (Hantzsch-Widman) nomenclature for monocyclic, fused ring and bridged heterocyclic systems. Aromatic heterocycles: Classification (structural type) Aromaticity, bond lengths, <sup>1</sup>H NMR, resonance energy, charge distribution, reactivity, tautomerism. Non-aromatic heterocycles: Bond angle and torsional strains and their consequences in small ring heterocycles. Small ring heterocycles: Three-membered and four-membered heterocycles-synthesis and reactions of aziridines, oxiranes, azetidines.

**Unit-II**

Methods of synthesis and reactions including mechanism (addition on nitrogen: protonation, *N*-alkylation, *N*-acylation; reactions with electrophilic and nucleophilic reagents) of the following five - membered 1,2- and 1,3-heterocycles: pyrazole, imidazole, oxazole, thiazole; their basic character. Reactions with oxidizing and reducing agents. Synthesis and reaction of quarternary 1,3-azolium and 1,3-azole *N*-oxide.

Methods of synthesis and reactions including mechanism of the following six-membered heterocycles: purines and pyrimidines. Methods of synthesis and reactions including mechanism of Indoles, quinolines and isoquinolines.

**Unit-III**

Disconnection Approach: An introduction of synthons and synthetic equivalents, general principles of the disconnection approach, functional group interconversions, the importance of order of events in organic synthesis, one group C-X and two group C-X disconnections, one group C-C disconnections- alcohols and carbonyl compounds, chemoselectivity, reversal of polarity, amine synthesis.

**Unit-IV**

Two group C-C disconnection- 1,3- and 1,5-difunctionalized compounds. Domino reactions. Principle of protection of alcoholic, amino, carbonyl and carboxylic groups. Disconnection approach toward the synthesis of Morphine, Longifolene, Juvabione and its relative merits and demerits.



**Suggested Readings:**

1. Gilchrist, T. L., Heterocyclic Chemistry, Prentice Hall, 1997.
2. L.A. Paquette, Principles of Modern Heterocyclic Chemistry, W.B. Benjamin, Inc., 1978.
3. Joule, J. A. and Mills, K. Heterocyclic Chemistry, Fifth Edition, Wiley, 2010.
4. S. Warren, Organic Synthesis, The disconnection Approach, John Wiley & Sons, 2004
5. Heterocyclic chemistry by Gupta and Gupta, Wiley Intersciences.
6. R. K. Bansal, Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms, Wiley Eastern Ltd., 1990.
7. B.M. Acheson, An Introduction to the Chemistry of Heterocyclic Compounds, Interscience, 2nd Ed., 1975.
8. Eicher, T.; and Hauptmann, S.; The chemistry of Heterocycles, Wiley-VCH, Weinheim, 2003.
9. S. Warren, Designing Organic Synthesis, Wiley.
10. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996
11. E. J. Corey and X-M. Cheng, -The logic of chemical synthesis, John-Wiley & Sons, New York, 1989.
12. K. C. Nicolaou, Classics in Total Synthesis of Natural Products, Vol. I (1996) & Vol. II (2003).

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 403(c): Advanced Organic Synthesis and Organic Materials**  
**(Organic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

*Note: There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Organocatalysis in Organic Synthesis: Introduction. Enamine catalysis: Aldol and Mannich type reactions,  $\alpha$ -heteroatom functionalization, direct conjugate additions via enamine activation. Iminium catalysis: the catalysis concept, cycloaddition reactions, 1,4-addition reactions, transfer hydrogen, cascade reactions. Ammonium ions as chiral templates: Homogeneous catalysis with chiral quaternary ammonium salts, Heterogeneous catalysis- chiral phase transfer catalysis. Morita-Baylis-Hillman reaction: addition of ketones and aldehydes to activated olefins, asymmetric MBH reactions. Organocatalytic oxidation and reduction reaction.

**Unit-II**

Multi-component reactions: Mechanism and synthetic application of Ugi, Passerini, Biginelli and Mannich reactions.

Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, mechanism and applications.

**Unit-III**

Asymmetric synthesis: Enantiomer excess, % enantioselectivity, optical purity, % diastereomeric excess and % diastereoselectivity.

Classification of asymmetric reactions: (a) Substrate controlled asymmetric synthesis: Nucleophilic additions to chiral carbonyl compounds. 1, 2- asymmetric induction, Cram's rule and Felkin-Anh model.

(b) Chiral auxiliary controlled asymmetric synthesis:  $\alpha$ -Alkylation of chiral enolates, imines and hydrazones. 1, 4-Asymmetric induction and Prelog's rule. Use of chiral auxiliaries in Diels-Alder and Cope reactions. (c) Chiral reagent controlled asymmetric synthesis: Asymmetric reductions using BINAL-H. Asymmetric hydroboration using (Ipc)<sub>2</sub>BH. (d) Chiral catalyst controlled asymmetric synthesis: Asymmetric hydrogenations using chiral Wilkinson biphosphine and Noyori catalysts.

### Unit-IV

Organic Materials: Molecular electronics: molecular materials for electronics and molecular scale electronics: Molecular properties, molecular arrangement and molecular interactions, piezoelectric and pyroelectric organic materials; molecular magnets based on transition metal complexes and organic ferromagnets, organic non-linear optical materials: photochromic organic materials and their classes; conducting polymers: polyacetylene, polypyrrole, polyaniline and polythiophene; conductive charge transfer materials: TTFTCNQ, metal–dithiolate systems, fullerenes. Langmuir-Blodgett films, molecular electronic logic and architectures.

#### Suggested Readings:

1. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, Chapter 30, Oxford University Press, Oxford (2001).
2. S. Warren, Designing of organic synthesis – (Wiley)
3. W. Carruthers, Modern Methods of Organic Synthesis, Cambridge University Press, 1996.
4. Robert E. Gawley, J. Aube, Principles of Asymmetric Synthesis Pergamon Title, Annotated Ed. 2004,
5. Nogradi, M.; Stereoselective Synthesis: A Practical Approach, Wiley-VCH, 2nd Ed. 1994.
6. List. B. et.al. Asymmetric Organocatalysis, Springer 1st Ed. 2010
7. F. A. Carey and R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edition, Springer, 2009
8. B. M. Trost and I. Fleming, Comprehensive Organic Synthesis, Pergamon Press, 1992
9. R. O. C. Norman and J. M. Coxon Principles of Organic Synthesis 3rd edition, Nelson Thornes, 2005
10. Roderick Bates, Organic synthesis using transition metals- (Wiley)
11. J. M. Swan and D. C. Black, Organometallics in organic synthesis – (Chapman and Hall)
12. J.S. Bindra and R. Bindra , Creativity in Organic Synthesis, Academic Press, NY (1975).
13. T. Hudlicky and J. W. Reed, –The way of synthesis| , Wiley-VCH, 2007.
14. E. J. Corey and X-M. Cheng, –The logic of chemical synthesis, John-Wiley & Sons, New York, 1989.
15. P.J. Vander Put, Inorganic Chemistry of Materials, Plenum Press, New York, 1998.
16. M.C. Petty, M.R. Bryce and D. Bloor, Editors An Introduction to Molecular Electronics, Edward Arnold, London 1995.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE 404(c): Chemistry of Natural Products**  
**(Organic Chemistry Specialization)**

Maximum Marks: 100  
Theory Examination: 80  
Internal Assessment: 20  
Max. Time: 3 hrs.

**Note:** *There shall be nine questions in all. Question no. 1 shall be compulsory, consisting of eight short answer type questions covering the entire syllabus. Two questions will be asked from each unit. Student will have to attempt one question from each unit. Each question shall carry equal marks.*

**Unit-I**

Alkaloids: Definition, nomenclature and physiological action, occurrence, isolation Structure elucidation of alkaloids – a general account; degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following: Ephedrine, (+)-Conine, Nicotine, Quinine, and Reserpine.

**Unit-II**

Terpenoids: Classification, general aspects of structure determination of terpenoids, biogenetic isoprene rule. Structure, stereochemistry, synthesis and biogenesis of Geraniol,  $\alpha$ -terpeneol,  $\alpha$ -pinene, camphor. Carotenoids: General method of structure elucidation, biosynthesis and synthesis of  $\beta$ -carotene, Vitamin A and Abietic acid.

**Unit-III**

Steroids: Isolation, nomenclature basic skeleton, Diel's hydrocarbon, stereochemistry, structural elucidation with special reference to Cholesterol, Bile acid and cardiac glycosides.

Methods for the following conversions:

Cholesterol to Testosterone

Cholesterol to Progesterone.

Biogenesis of steroids and correlation with terpenoids.

Prostaglandins: Introduction, nomenclature and biological role of prostaglandins. Synthesis of PGE<sub>2</sub> and PGF<sub>2 $\alpha$</sub>

**Unit-IV**

Natural Pigments: Occurrence nomenclature and general methods of structure determinations, isolation and synthesis of Cyanin, Quercetin, Diadzein, and Chrysin. Biosynthesis of Flavonoids: Acetate path way and shikimic acid pathway.

Porphyryns: Structure elucidation of chlorophyll, General structural features of Haemoglobin (not structure elucidation).

**Suggested Readings:**

1. I. L. Finar, Organic Chemistry, Vol. II, 5th Edition (1975) Reprinted in 1996, ELBS and Longman Ltd, New Delhi.
2. J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, Chapter 30, Oxford University Press, Oxford (2001).
3. Nitya Anand, J.S. Bindra and S. Ranganathan, Art in Organic Synthesis, 2nd Edition (1970), Holden Day, San Francisco.
4. S.W. Pelletier, Chemistry of the Alkaloids, Van Nostrand Reinhold Co., New York (1970).
5. K.W. Bentley, The Alkaloids, Vol. I., Interscience Publishers, New York (1957).
6. J.W. Apsimon, Total Synthesis of Natural Products, Vol. 1-6, Wiley-Interscience Publications, New York (Vol. 1, 1973).
7. K. C. Nicolaou, Classics in Total Synthesis of Natural Products, Vol. I (1996) & Vol. II (2003).
8. J.S. Bindra and R. Bindra, Creativity in Organic Synthesis, Academic Press, NY (1975).
9. J.S. Bindra and R. Bindra, Prostaglandins Synthesis, Academic Press. Inc., New York, London (1977).
10. T. Hudlicky and J. W. Reed, -The way of synthesis, Wiley-VCH, 2007.

**M.Sc- Chemistry**  
**Semester-IV**

**CHE-406 Practical- IV**  
**Organic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Multi-step organic synthesis and applications of spectroscopic techniques to determine the structures of the compounds prepared.
  - (i) Synthesis of 2-chloro-4-bromo-6-iodoaniline from aniline.(Book 1, pp 292-299)
  - (ii) Synthesis of anthranilic acid from phthalimide. (Book 2, pp 898-899)
  - (iii) Reduction of 3-nitroacetophenone using i) NaBH<sub>4</sub> ii) using Sn and HCl.(Modern projects and experiments in organic chemistry)
  - (iv) Michael addition of aniline to benzalacetophenone. (Book 1, p 247)
  - (v) Or any other relevant synthesis
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**CHE-407 Practical- V**  
**Organic Chemistry Practical**

Max. Marks: 50  
Time: 6 hrs.

1. Multi-step organic synthesis and applications of spectroscopic techniques to determine the structures of the compounds prepared.
  - (i) Conversion of benzalacetophenone to its oxime and its transformation to amide and oxazole derivatives. (Book 1, pp 242-247, Book 3 pp 361-365)
  - (ii) Synthesis of p-aminobenzenesulfonamide. (Book 1, pp 275-289)
  - (iii) Synthesis of Methyl n-pentyl ketone from ethyl acetoacetate. (Book 2, pp 620-621)
  - (iv) Synthesis of triphenylcarbinol from bromobenzene. (Book 2, pp 540-541)
  - (v) Or any other relevant synthesis
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**CHE-408 Practical- VI**  
**Organic Chemistry Practical**Max. Marks: 50  
Time: 6 hrs.

1. Preparation and characterization organic compounds prepared in two and three steps.
  - (i) Synthesize (a) 2,4-dinitro-1-chlorobenzene from chlorobenzene, (b) mixture of o- and p-nitrophenols from phenol and (c) p-nitroacetanilide from acetanilide and make comparison of the reactivity of various substrates and reaction conditions used for performing nitration in each experiment. (Book 2, pp 978-979, 919-20)
  - (ii) Synthesis of benzalacetophenone by condensation of benzaldehyde with acetophenone and study its bromination and subsequent debromination. (Book 1, pp242-247, Book 3 pp 361-365)
  - (iii) The epoxidation of benzalacetophenone to its epoxide and study its reactivity towards hydroxyl ion. (Book 3, pp 363-364).
  - (iv) Nitration of o-chlorobenzoic acid and o-chloroacetanilide –separation and identification of isomers
  - (v) Or any other relevant experiment
2. Viva-Voce (05 Marks)
3. Note Book (05 Marks)

**Suggested readings:**

1. An Introduction to Modern Experimental Organic Chemistry, R.M. Roberts, Gilbert, L.B. Rodewald and A.S. Wingrove. Holt, Ranehart and Winston Inc., J.C New York.1969.
2. Vogel's Text Book of Practical Organic Chemistry, 5th Edition.
3. Laboratory Experiments in Organic Chemistry, R. Adams, J.R. Johnson and C.F. Wilcox, The Macmilan Limited, London, 1970