YBN UNIVERSITY
Established by the Act of Government of Jharkhand Act 15, 2017
Gazette Notification No. 505, Dated 17th July 2017
As per Section 2(f) of UGC Act. 1956

# YBN UNIVERSITY, RANCHI (JHARKHAND)

## UNIVERSITY DEPARTMENT OF CHEMISTRY

## SCHOOL OF SCIENCE

# M.Sc. Programme in Chemistry
**(Based on CBCS Pattern)**

**Detailed Guideline and syllabus for two years(24 Months) M.Sc.**

**Programme in Chemistry 2020 onwards**

**APPROVED BY**
**THE BOARD OF STUDIES**
**UNIVERSITY DEPARTMENT OF CHEMISTRY**
**SCHOOL OF SCIENCE**
**YBN UNIVERSITY, RANCHI (JHARKHAND)**

**Our Vision**

The Vision of the Department of Chemistry is to generate and disseminate Chemistry education among its pupils such that at individual level, a Chemistry graduate should be inspired with a sense of curiosity and wonder about the fundamental nature of the world around the student, be empowered with the ability to make decisions about their own lives and critically evaluate scientific and technological developments that impact society and lastly be equipped with the knowledge and skills to pursue further study and rewarding careers in the chemical sciences and a wide range of related fields.

**Our Mission**

1: To represent a clear framework or narrative that gives a coherent 'big picture' of chemistry as a subject, explains why it matters, and shows how different areas of content are connected.
2: To prepare competitive and professional graduates within an innovative and intellectually stimulating environment, support other academic programs at YBN University by offering quality chemistry learning experiences, conduct basic and applied research of national and international impact.
3: To advance knowledge platform that supports an invent-and-design culture in graduate and undergraduate chemistry education and that empowers students to address and solve challenges of global significance.
4: To reach out to our future thought leaders—students of all backgrounds from pre-college to doctoral candidates—to share the power of chemistry to create new knowledge directed at the major unmet needs of our time.

**Introduction to the Program:**

M. Sc. in Chemistry is a 2-year full-time postgraduate course at YBN University, RANCHI, JHARKHAND that is dedicated to providing the best and highest quality of education to the aspiring students in this domain. The program has been diligently crafted to make the students have a foretaste of the future. With the ever-increasing demand of M. Sc. in Chemistry more number of students are trying to enroll themselves in this branch so that they enjoy great career and life ahead waiting for them. The course will make you ever ready to face modern world challenges and requirements with utmost confidence.
The program of M. Sc. in Chemistry is designed to render the basic and advance study in Chemistry for the aspiring students. School of Science, YBN UNIVERSITY, RANCHI offers specialization in Inorganic Chemistry, Organic Chemistry, Physical Chemistry, Analytical Chemistry, Atmospheric Chemistry, Bio-inorganic Chemistry, Bio-organic Chemistry, Bio-physical Chemistry, Nano-chemistry, and lot more
With a fine balance between the depth through theoretical learning and the intellectual exposure through practical learning and hands-on experience with field-trips and laboratory practicals the students gain wholesome development.

**Program Specific Objectives:**

1. To educate and prepare post graduate students from rural and urban area who will get employment on large scale in academic institutes, R & D and Quality control

laboratories of Indian chemical/pharmaceutical industries as well as multinational and forensic Laboratories.

2. To provide students with broad theoretical and applied background in all specialization of Chemistry with emphasis on qualitative and quantitative technique.
3. To provide broad common frame work of syllabus to expose our young graduates to the recent and applied knowledge of interdisciplinary branches of chemistry involving applied organic, inorganic, physical, analytical, industrial, pharmaceutical, polymer, Nano science & technology.
4. To conduct lesser written tests and to encourage on non-written tests.
5. To focus on encouraging students to conduct various academic activities like midterm tests, online tests, open book tests, tutorial, surprise test, oral, seminar, assignments and seminar presentation.

**Program Outcomes (PO):**

**PO1: Creative Thinking:** Students will be able to think creatively (divergently and convergent) to propose novel ideas in explaining facts and figures or providing new solution to the problems in chemistry. The skills of observations and drawing logical inferences from the scientific experiments will also be developed.

**PO2: Interdisciplinary Approach:** Students will realize how developments in any science subject helps in the development of other science subjects and vice-versa and how interdisciplinary approach helps in providing better solutions and new ideas for the sustainable developments. Also the knowledge of subjects in other faculties such as humanities, performing arts, social sciences etc. can have greatly and effectively influence which inspires in evolving new scientific theories and inventions.

**PO3: Personality Development:** Students will imbibe ethical, moral and social values in personal and social life leading to highly cultured and civilized personality. They will also realize that pursuit of knowledge is a lifelong activity and in combination with untiring efforts and positive attitude and other necessary qualities leads towards a successful life.

**PO4 Skills in research and industrial field:** Students will build a scientific temper and will be able to learn the necessary skills to succeed in research or industrial field. In addition they will acquire the skills in handling scientific instruments, planning and performing in laboratory experiments.

**PO5 Communication Skills:** Students will develop various communication skills such as reading, listening, speaking, etc., which we will help in expressing ideas and views clearly and effectively.

**PO6 Environmental monitoring:** Students will be able to understand the **e**nvironmental issues Global warming, Climate change, Acid rain, Ozone depletion and will create awareness in society .

**Program Specific Outcomes (PSO):**

**PSO-1** Students will understand the basic concepts, fundamental principles, and the scientific theories related to various scientific phenomena and their relevancies in the day-to-day life. They will also be able to acquire knowledge about the fundamentals and applications of chemical and scientific theories.

**PSO-2** Students will find that every branch of science and technology is related to Chemistry. They will develop scientific outlook not only with respect to science subjects but also in all aspects related to life.

**PSO-3** Students will become familiar with the different branches of chemistry like analytical, organic, inorganic, physical, environmental, polymer and biochemistry. They will also learn to apply appropriate techniques for the qualitative and quantitative analysis of chemicals in laboratories and in industries.

**PSO-4** The student will acquire knowledge of Chemical Thermodynamics, Kinetics, Electrochemistry, Atomic Structure, Organic Chemistry, Spectroscopy and Skill in Industrial Chemistry.

**PSO-5** Viewing chemistry as a tool the developing mind and critical attitude and the faculty of logical reasoning that is prepared to serve in diverse fields.

**PSO-6** Students will gain a thorough Knowledge in the subject to be able to work in projects at different research as well as academic institutions.

**Programme Eligibility:**

Passed B.Sc(Hons.) examination with Chemistry with 50% marks.

## GENERAL GUIDELINES

1. M.Sc. Course in Chemistry shall be of two years duration.

2. There shall be semester wise examination.

3. There shall be four semester (04) in two years, Semester-I and Semester-II in first year ($1^{st}$ year) and Semester-III and Semester-IV in the second year ($2^{nd}$ year).

4. There shall be three theory papers of 100 marks each of THREE HOURS duration and one practical exam of 100 marks of SIX HOUR duration in each Semester-I, II & III. In Semester-IV, there will be one PROJECT WORK of 100 MARKS. There shall be a Mid Term Examination also in each Semester of 30 marks in each theory papers.

5. There shall be 11 theory papers, 4 practical papers and 1 Project Work altogether.

6. There shall be THREE GROUPS of optional elective paper, out of which student has to elect ONE GROUP.

   GROUP OF ELECTIVE PAPERS:

   Group-A : INORGANIC CHEMISTRY
   Group-B : ORGANIC CHEMISTRY
   Group-C : PHYSICAL CHEMISTRY

7. Each theory paper in each END SEMESTER EXAMINATION shall carry SEVENTY (70) as FULL MARKS.

8. There shall be MID SEMESTER EXAMINATION/ INTERNAL EVALUATION in the middle of each Semester carrying THIRTY (30) as FULL MARKS.

9. There shall be total EIGHT (08) questions in each End-Semester Examinations. Examinees are required to answer any FIVE (05) questions out of EIGHT (08).

10. The duration of End-Semester Examination shall be of THREE (03) HOURS in each theory paper of each Semester.

# Course Structure for M.Sc. Programme in Chemistry

| SEM | COURSE OPTED | Paper | Distribution of Marks | | | |
|---|---|---|---|---|---|---|
| | | | END SEM | MID SEM | PRACTICAL / PROJECT | TOTAL |
| I | FC (Compulsory) – (FC-I) | 1 | 70(50+20) | 30 | - | 100 |
| | Core Course – 1 (CC-1) | 2 | 70(50+20) | 30 | - | 100 |
| | Core Course – 2 (CC-2) | 3 | 70(50+20) | 30 | - | 100 |
| | Core Course (P) – 3 [CC (P)-3] | 4 | - | - | 100 | 100 |
| II | Elective Course (SE) (EC-1) | 5 | 70(50+20) | 30 | - | 100 |
| | Core Course – 4 | 6 | 70(50+20) | 30 | - | 100 |
| | Core Course – 5 | 7 | 70(50+20) | 30 | - | 100 |
| | Core Course (P) – 6 [CC (P)-6] | 8 | - | - | 100 | 100 |
| III | Core Course – 7 | 9 | 70(50+20) | 30 | - | 100 |
| | Core Course – 8 | 10 | 70(50+20) | 30 | - | 100 |
| | Elective (GE/DC) (EC-2) | 11 | 70(50+20) | 30 | - | 100 |
| | Elective Course (P) – 3 [EC (P)-3] | 12 | - | - | 100 | 100 |
| IV | Core Course – 9 | 13 | 70(50+20) | 30 | - | 100 |
| | Elective (GE/DC) (EC-4) | 14 | 70(50+20) | 30 | - | 100 |
| | Elective Course (P) – 5 [EC (P)-5] | 15 | - | - | 100 | 100 |
| | Project | 16 | - | - | 100 | 100 |

## Semester-wise Distribution of Course

| SEM | COURSE | CREDIT | Hrs./Week |
|---|---|---|---|
| I | FC (Compulsory) – (FC-I) | 5 | 5(L)+1(T) |
| | Core Course – 1 (CC-1) | 5 | 5(L)+1(T) |
| | Core Course – 2 (CC-2) | 5 | 5(L)+1(T) |
| | Core Course (P) – 3 [CC (P)-3] | 5 | 10 |
| II | Elective Course (SE) (EC-1) | 5 | 5(L)+1(T) |
| | Core Course – 4 | 5 | 5(L)+1(T) |
| | Core Course –5 | 5 | 5(L)+1(T) |
| | Core Course (P) – 6 [CC (P)-6] | 5 | 10 |
| III | Core Course – 7 | 5 | 5(L)+1(T) |
| | Core Course – 8 | 5 | 5(L)+1(T) |
| | Elective (GE/DC) (EC-2) | 5 | 5(L)+1(T) |
| | Elective Course (P) – 3 [EC (P)-3] | 5 | 10 |
| IV | Core Course – 9 | 5 | 5(L)+1(T) |
| | Elective (GE/DC) (EC-4) | 5 | 5(L)+1(T) |
| | Elective Course (P) – 5 [EC (P)-5] | 5 | 5(L)+1(T) |
| | Project | 5 | 10 |

| COURSE STRUCTURE OF M.Sc CHEMISTRY FIRST SEMESTER | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Course Details | | | | External Assessment | | Internal Assessment | | | | Credit Distribution | | | Allotted Credits |
| Course Code | Course Type | Course Title | Total Marks | Major | | Minor | | Sessional | | L | T | P | Subject wise Distribution |
| | | | | Max. Marks | Min. Marks | Max. Marks | Min. Marks | Max. Marks | Min. Marks | | | | |
| 1Y2CHE101 | Foundation Course(Compulsory) | General Chemistry | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE102 | Core Course-I | Transition Metal Complex | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE103 | Core Course-II | Reaction Mechanism in Organic Chemistry | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE104P | Core Course-III Practical | Core Course Practical | 100 | 50 | 17 | 20 | 07 | 30 | 10 | - | - | 10 | 5 |
| | Grand Total | | 400 | | | | | | | | | | 20 |

**Minimum Passing Marks are equivalent to Grade D**
**Lectures T- Tutorials P- Practical, Major- Term End Theory Exam**
**Minor- Pre University Test**
**Sessional weightage – Attendance 50%, Three Class Tests/Assignments 50%**

# M.Sc. Semester-1
# FC – Compulsory (FC-1)
# Course Code : 1Y2CHE101
## (General Chemistry)

**Full Marks: 50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Nature of Bonding in Main Group Inorganic Compounds 15 Hrs**

VSEPR, Chemical Bonding- VSEPR model, Walsh diagrams (tri-atomic molecules of type $AH_2$), dπ-pπ bonds, shapes of molecules-$ClF_3$, $ICl_4^-$, $TeF_5^-$, $I_3^-$, $TeCl_6^{2-}$, $XeF_6$, $SbCl_6^{3-}$, $IF_7$, $ReF_7$; Bent rules and energetics of hybridization; electronegativity and partial ionic character; Some simple reactions of covalently bonded molecules, Atomic Inversion, Berry Pseudorotation. Bonds-Multicenter, Synergic and Agostic bonding. Lattice energy: Born-Lande equation, Kapustinskii equation; polarizability and partial covalent character, radius-ratio rules, structures of simple solids, Zintl-isoelectronic relationship in solids. Molecular orbital theory: MO diagrams of heteronuclear diatomic (CO and NO).

**II Crystal Structure of Ionic Compounds 15 Hrs**

Ionic crystals and their structures, radius ratio rule, effect of polarization on crystals. Covalent structure type- Sphalerite & Wurtzite, Geometry of simple crystal AB type: NaCl, CsCl & NiAs, reasons for preference for a particular structure in above AB type of compounds. $AB_2$ type: Fluorite, antifluorites, Rutile structures. $Li_2O$, $Na_2O$, $CdCl_2$, $CdI_2$ structures. Defects in Solids: Point defects, Line defects and Plane defects. Ternary Compounds $ABO_3$ type: Perovskite, Barium titanate, lead titanate, $CaTiO_3$, $FeTiO_3$, Tolerance factor, charge neutrality and deviation structures. $AB_2O_4$ type-compounds: Normal & inverse, 2-3 and 4-2 spinel, site preferences in spinel, distorted spinel, Factors causing distortion in spinel.

**III Unifying Principles 10 Hrs**

Electromagnetic radiation, interaction of electromagnetic radiation with matter-absorption, emission, transmission, reflection, refraction, dispersion, polarisation and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, results of the time dependent perturbation theory, transition moment, selection rules, intensity of spectral lines, Born-Oppenheimer approximation, rotational, vibrational and electronic energy levels.

**V Surface Chemistry 20 Hrs**

Surface chemistry, types of adsorption curves, experimental methods of determining adsorption, Freundlich adsorption isotherm and its derivation, Traube's rule, Langmuir adsorption isotherm and its derivation, BET isotherm for multilayers and its derivation, properties of BET equation, methods for Determining surface area, heat of adsorption and its calculation, entropy of adsorption, Polanyi's potential theory, statistical treatment of Langmuir's adsorption isotherm, kinetics of gaseous reactions on solid surface: unimolecular and bimolecular surface reaction, temperature dependence of surface reactions, electrocapillarity, electrokinetic effects. Gibb's adsorption equation and its derivation, verification of Gibb's adsorption equation, surface excess.

**V Nuclear Chemistry** **10 Hrs**

Nuclear Chemistry-The atomic nucleus-elementary particles, quarks, classification of nuclides based on Z and N values, nuclear stability, nuclear potential, binding energy. Nuclear Models: Shell model-salient features, forms of the nuclear potential, filling of orbitals, nuclear configuration, Liquid drop model, Fermi gas model, Collective model and Optical model. Radioactivity, radioactive decay kinetics, Parent-daughter decay-growth relationship-secular and transient equilibria, theories of $\alpha$, $\beta^-$, $\beta^+$ and $\gamma$-decay, internal conversion, Auger effect.

**Reference Books**


1. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
4. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
5. Physical Chemistry- Waller J. Moore
6. Physical Chemistry - P.W. Atkins
7. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).
8. Essentials of Nuclear Chemistry, 4th edition; H. J. Arniker, NAIL publishers (1995); Chapters 1, 3 and 4.
9. Nuclear and Radioactive Chemistry: Friedlander, Kennedy and Miller; Chapters 8 and 9.
10. Solid State Chemistry, D.K. Chakraborty (New Age Int. Publication)
11. Physical Chemistry of Surfaces, A. W. Adamson, Interscience Publisher Inc., New York (1967).
12. Surface Chemistry: Theory and Applications, J. J. Bikerman, Academic Press. New York (1972).

# M.Sc. Semester-II
# Core Course – 1 (CC-1)
# Course Code : 1Y2CHE102
## (Transition Metal Complexes)

**Full Marks:**
**50+20+30**
**Total Lecturer: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Reaction Mechanism of Transition Metal Complexes 25 Hrs**

(A) Energy profile of a reaction, reactivity of metal complexes, Reaction mechanism-Labile, inert, stable and unstable complexes. Classification of mechanisms - Energy profile of reactions having different mechanisms. Kinetic application of valence bond and crystal field theories, Kinetics of octahedral substitution, acid hydrolysis, base hydrolysis, conjugate base mechanism, direct and indirect evidences in favour of conjugate mechanism, anation reactions, reactions without metal ligand bond cleavage. Substitution reactions in square planar complexes - Factors affecting substitution, Reactivity of Platinum complexes: Influences of entering and leaving groups, Trans effect in the synthesis of complexes, Theories of trans-effect, Application of trans-effect in the synthesis of complexes. Mechanism of ligand substitution in octahedral complexes: Kinetics and Factors affecting substitution in octahedral complexes: Leaving group, Chelate and Metal effects. Redox reactions.

(B) Acid-Base catalysis: Acid catalysed aquation and anation reactions, acid hydrolysis, base hydrolysis, conjugate base hydrolysis, mechanism of acid hydrolysis and base hydrolysis stereochemistry of octahedral substitution, Replacement of coordinated water - Conjugate base mechanism, evidences in favour of the mechanism, application in the synthesis of platinum and cobalt complexes.

(C) Electron transfer reactions – Outer sphere electron transfer reaction, Marcus equation, Inner sphere electron transfer reaction, formation and rearrangement of precursor complexes, the bridging ligand, successor complexes, cross reactions and Marcus-Hush theory. Use of electron transfer reactions for the synthesis of complexes.

**II Stereochemistry of Transition Metals Complexes 10 Hrs**

Stereochemical aspects - Stereoisomerism in inorganic complexes, isomerism arising out of ligand distribution and ligand conformation, chirality and nomenclature of chiral complexes.

**III Stability of Transition Metals Complexes 10 Hrs**

Stability of complexes - Factors affecting stability of complexes, thermodynamic aspects of complex formation, Stepwise and overall formation constants, stability correlations, statistical and chelate effects, Determination of stability constant - Polarographic, photometric and potentiometric methods.

**IV Electronic Spectra of Transition Metal Complexes 15 Hrs**

Spectroscopic ground states, selection rules, term symbols for $d^n$ ions, Racah parameters, Orgel, Correlation and Tanabe-Sugano diagrams for transition metal complexes ($d_1$-$d_9$

states). Spectra of 3d metal-aqua complexes of trivalent (V and Cr), divalent (Mn, Co and Ni) complexes and $CoCl_4^{2-}$. calculations of Dq, B and b parameters, Charge transfer spectra, spectroscopic method of assignment of absolute configuration in optically active metal chelates and their stereochemical information. Spectral properties of Lanthanide and Actinide metal complexes.

**V Magnetic Properties of Transition Metal Complexes 10 Hrs**

Magnetic properties of coordination compounds - Types of magnetic behaviour, magnetic susceptibility and its determination : Gouy, Faraday, and VSM method. Diamagnetic correction, orbital contribution, spin-orbital coupling, ferro- and antiferro- magnetic coupling, magnetic exchange coupling and spin-crossover. Anomalous magnetic moments and their explanation. Magnetic properties of Lanthanide and Actinide metal complexes.

**Reference Books**


1. Inorganic Chemistry IV edition; J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison; Wesley (1993).
2. Advanced Inorganic Chemistry, 6th edition; F. A. Cotton and G. Wilkinson.
3. Inorganic Chemistry, II edition, D. F. Shriver, P. W. Atkins and C. H. Langford, ELBS; Oxford University Press, 1994.
4. Concise Inorganic Chemistry, 5th edition; J. D. Lee (1996).
5. Inorganic Chemistry, 3rd Edition; Gary. L. Miessler and Donald . A. Tarr (2007).
6. PhysicaI Methods in Chemistry, R.S. Drago, Saunders College.
7. Chemisiry ol the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
8. Inorganic Electron Spectroscopy, A. B. P. Lever, Elsevier (1968)
9. Magnetochemistry, R.L. Carlin, Springer Vertag,
10. Electronic Absorption Spectroscopy and Related Techniques, D. N. Sathyanarayana, University Press (2001).
11 Comprehensive Coordination Chemistry eds., Q. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.

# M.Sc. Semester-I
# Core Course – 2 (CC-2)
# Course Code : 1Y2CHE103
## (Reaction Mechanism in Organic Chemistry)

**Full Marks:**
**50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Nature of Bonding in Organic Molecules** **15 Hrs**

Aromaticity in benzenoid and non-benzenoid compounds(including annulenes and heterocyclic compounds), alternant and non-alternant hydrocarbons, Huckel's rule, energy level of 7-molecular orbitals, azulene, annulenes, anti-aromaticity, π- aromaticity, homo-aromaticity, PMO approach.
Bonds weaker than covalent-addition compounds, crown ether complexes and cryptands, inclusion compounds, cyclodextrins, catenanes and rotaxanes.

**II Stereochemistry** **15 Hrs**

Conformational analysis of cycloalkanes, decalins, effect of conformation on reactivity, conformation of sugars, steric strain due to unavoidable crowding.
Elements of symmetry, chirality, molecules with more than one chiral center, threo and erythro isomers, methods of resolution, optical activity, enantiotopic and diastereotopic atoms, groups and faces. Stereospecific and stereoselective synthesis. Asymmetric synthesis. Optical activity in the absence of chiral carbon (biphenyls, allenes and spiranes), chirality due to helical shape. Stereochemistry of the compounds containing nitrogen, sulphur and phosphorus. Regeoselectivity.

**III Aliphatic Nucleophilic Substitution** **10 Hrs**

The $S_N2$, $S_N1$, mixed $S_N1$ and $S_N2$ and SET mechanisms. The neighbouring group mechanism, neighbouring group participation, anchimeric assistance.
Classical and nonclassical carbocations, phenonium ions, norbornyl system, common carbocation rearrangements.
The $S_Ni$ mechanism.Nucleophilic substitution at an allylic, aliphatic trigonal and a vinylic carbon. Reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, phase transfer catalysis and ultrasound, ambident nucleophile, regioselectivity.

**IV Aromatic Nucleophilic Substitution** **05 Hrs**

The $S_NAr$, $_{SO,}$ benzyne and $_{SRO}$ mechanisms. Reactivity - effect of substrate structure, leaving group and attacking nucleophile. The von Richter, Sommelet-Hauser, and Smiles rearrangements.

**V. Aliphatic Electrophilic Substitution : 05 Hrs**

Bimolecular Mechanisms- $S_E2$ & $S_E$. The Electrophilic Substitution reaction accompanied by double bond shifts. Effect of substrates, leaving group and the solvent polarity on the reactivity.

**VI Aromatic Electrophilic Substitution** **10 Hrs**

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. Diazo-coupling reaction, Vilsmeir reaction, Gattermann-Koch reaction.

**VII Free Radical Reactions** **10 Hrs**

Types of free radical reactions, free radical substitution mechanism, mechanism at an aromatic substrate, neighbouring group assistance. Reactivity for aliphatic and aromatic substrates at a bridgehead. Reactvity in the attacking radicals. The effect of solvents on reactivity. Allylic halogenation (NBS), oxidation of aldehydes to carboxylic acids, auto-oxidation, coupling of alkynes and arylation of aromatic compounds by diazonium salts. Sandmeyer reaction. Free radical rearrangement. Hunsdiecker reaction.

**Reference Books**


1. Advanced Organic Chemistry-Reactions, Mechanism and Structure, Jerry March, John Wi1ey.
2. Advanced Organic Chernistry, 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. Pericyclic Reactions, S. M. Mukherji, Macmillan, India.
7. Reaction Mechanism in Organic Chemistry, S. M. Mukherji and S. P. Singh, Macmillan.
8. Stereochemistry of Organic Compounds, D. Nasipuri, New Age international.

# M.Sc. Semester-I
# Core Course (P) – 3 [CC(P)-3]
# Course Code : 1Y2CHE104P

**Full Marks: 100**
**Pass Marks: 34**
**Time: 06 Hrs**

Two questions are to be set.

**I Estimation of the following**

(i) Magnesium by EDTA (Volumetrically)
(ii) Zinc by Potassium ferrocyanide (Volumetrically)
(iii) Nickel by Dimethylglyoxime (Gravimetrically)
(iv) Managnese in steel by Sodium bismuthate method.

**II Preparation of organic compounds using methods not involving more than two steps:**

(i) Preparation of Methyl Orange
(ii) Preparation of Martius yellow
(iii) Preparation of p-Nitro aniline from Acetanilide
(iv) Preparation of Cinnamic acid from Benzaldehyde

**III Estimation of**

(i) Glucose using Fehling's solution
(ii) Carbonyl group using 2,4-Dinitrophenyl hydrazine

**Practical-1: 50 Marks, Note Book:20 Marks, Viva: 30 Marks.**

| COURSE STRUCTURE OF M.Sc CHEMISTRY SECOND SEMESTER | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Course Details | | | | External Assessment | | Internal Assessment | | | | Credit Distribution | | | Allotted Credits |
| Course Code | Course Type | Course Title | Total Marks | Major | | Minor | | Sessional | | L | T | P | Subjectwise Distribution |
| | | | | Max. Marks | Min. Marks | Max. Marks | Min. Marks | Max. Marks | Min. Marks | | | | |
| 1Y2CHE201 | Elective Course-I | Elective Course | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE202 | Core Course-IV | Quantum Chemistry & Chemical Dynamics | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE203 | Core Course-V | Group Theory & Spectroscopy | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE204P | Core Course VI-Practical | Core Course Practical-Physical Chemistry | 100 | 50 | 17 | 20 | 07 | 30 | 10 | - | - | 10 | 5 |
| | Grand Total | | 400 | | | | | | | | | | 20 |

**Minimum Passing Marks are equivalent to Grade D**
**Lectures T- Tutorials P- Practical, Major- Term End Theory Exam**
**Minor- Pre University Test**
**Sessional weightage – Attendance 50%, Three Class Tests/Assignments 50%**

# M.Sc. Semester-II
# Elective Course (SE) (EC-1)
# Course Code : 1Y2CHE201
# Introduction to Computers for Chemist

**Full Marks: 50+20+30**
**Total Lecture :70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Introduction to Computers and Computing** **10 Hrs**

Basic structure and functioning of computers with a PC as an illustrative example. Memory, I/O devices. Secondary storage. Computer languages. Operating systems with DOS as an example. Introduction to UNIX and WINDOWS. Data Processing, principles of programming. Algorithms and flow-charts.

**II Computer Programming in C Language** **20 Hrs**

Elements of the Computer Language Constants and variables and data types. Operators and Expressions, Arithmetical, Relational, Logical, Assignment, Increment and Decrement operators. Input and output statements. Branching statements such as (if-else, goto, switch) statements. Decision making and looping (while, for, do).Arrays (one dimensional and two dimensional arrays).Sorting of data in an array. Function (user defined functions).

**III Programming in Chemistry** **25 Hrs**

Development of small computer codes involving simple formulae in chemistry, such as vander Waals equation, pH titration, kinetics, radioactive decay. Evaluation of lattice energy and ionic radii from experimental data. Linear simultaneous equations to solve secular equations within the Huckel theory. Elementary structural features such as bond lengths, bond angles, dihedral angles etc. of molecules extracted from a database such as Cambridge data base.

**IV Use of Computer Programmes** **15 Hrs**

The students will learn how to operate a PC and how to run standard programmes and packages. Execution of linear regression, X-Y plot, numerical integration and differentiation as well as differential equation solution programmes. Monte Carlo and Molecular dynamics. Programmes with data preferably from physical chemistry laboratory. Packages- MS-Word, MS-Excel, ORIGIN, MATLAB.

**Books Suggested**


1 Comdex Computer Course kit (XP Edition), Vikas Gupta, Dreamtech, New Delhi
2. Fox Pro For DOS & Windows, R.K.Taxali, BPB Publication.
3. Programming in ANSIC, E. Balaguruswamy, Tata McGraw Hill
4. Computer for Chemist Bansal, Pragati Prakshan

**OR**

## Biochemistry [Course Code : 1Y2CHE201]

**Full Marks: 50+20+30**
**Total Lecturer: 70 Hours**

**Eight questions are to be set out of which five are to be answered selecting at least one question from each group.**

**Group A: Biophysical Chemistry**

**I Bioenergetics** **10 Hrs**

Standard free energy, entropy and chemical potential change in biochemical reactions. The effect of temperature and pH on $\Delta G_o$. Methods of determination of free energy changes. Relationship between Keq and $\Delta G_o$. Oxidation, reduction reaction and hydrolytic reactions in biological system, redox potential (electron-transfer reactions), free energy changes of oxidation-reduction reactions.

**II Enzymes and Mechanism of Enzyme Action** **15 Hrs**

Basic considerations. Proximity effects and molecular adaptation. Enzymes : Introduction and historical perspective, 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 Koshtand's induced fit hypothesis, concept and identification of active site by the use of inhibitors, affinity labeling and enzyme modification by site-directed mutagenesis. Enzyme kinetics, Michaelis-Menten and Lineweaver-Burk plots, reversible and irreversible Inhibition.

Transition-state theory, orientation and steric effect, acid-base catalysis, covalent catalysis, strain or distortion. Examples of some typical enzyme mechanisms for chymotrypsin, ribonuclease, lysozyme and carboxypeptidase A.

**Group B: Bioinorganic Chemistry**

**III Essential and trace metals ions in biological systems** **15 Hrs**

Biological functions of inorganic elements, biological ligands for metal ions. Coordination by proteins, Tetrapyrrole ligands and other macrocycle. Influence of excess and deficiency of V, Cr, Mn, Fe, Co, Cu,& Zn. Genetic defects in the absorption of trace elements. Regulation and storage of trace elements. Role of minerals. Toxic effects of metals. Metal storage, transport and biomineralization with respect to Ferritin, Transferrin and Siderophores, $Na^+/K^+$ pump. Role of Ca in transport and regulation in living cells. Medicinal use of metal complexes as antibacterial, anticancer, use of cis-platin as antitumor drug, antibiotics & related compounds. Metal used for dignosis and chemotherapy with particular reference to anti cancer drugs.

**IV Bioenergetics and Biochemistry of Dioxygen** **10 Hrs**

DNA polymerisation, glucose storage, metal complexes in transmission of energy; chlorophylls, photosystem I and photosystem II in cleavage of water. Model systems. Oxygen transport and oxygen uptake proteins- transport and storage of dioxygen, Heme proteins and oxygen uptake, Non-porphyrin systems-hemerythrin and hemocyanin, dioxygen binding, Structure and function of hemoglobin, myoglobin, hemocyanins and hemerythrin, Bohr effect, Hill equation, Perutz mechanism showing structural changes in porphyrin ring system. Oxygenation and deoxygenation. Role of distal and proximal histidine; Model complexes for

dioxygen binding. Synthetic complexes of iron, cobalt and copper. Cyanide poisoning and treatment. Vanadium storage and transport.

**Group C: Bioorganic Chemistry**

**V Kinds of Reactions Catalysed by Enzymes** **10 Hrs**

Nucleophilic displacement on a phosphorus atom, multiple displacement reactions and the coupling of ATP cleavage to endergonic processes. Mechanisms for phosphoryl transfer reactions, The mechanistic role of the coenzymes in living systems : (i) Biotin coenzyme in carboxylation reactions, (ii) Thiamine pyrophosphate (TPP) in decarboxylation, (iii) Coenzyme A (CoASH) in the transfer of acyl group, (iv) Vitamin B12 coenzymes in molecular rearrangement reactions and in the synthesis of methionine and methane.

**VI Co-Enzyme Chemistry** **10 Hrs**

Cofactors as derived from vitamins, coenzymes, prosthetic groups, apoenzymes. Structure and biological functions of coenzyme A, thiamine pyrophosphate, pyridoxal phosphate, $NAD_+$, $NADP_+$, FMN, FAD, lipolic acid, vitamin $B_{12}$. Mechanisms of reactions catalyzed by the above cofactors.

**Reference Books**


1. Introduction to Biophysical chemistry, R. Bruce Martin, McGraw-Hill, NY, 1964.
2. Physical Chemistry with applications to Biological systems, Ramond Chnag, Mc Millan publishing Co.inc, New York 1977.
3. Understanding Enzymes, Trevor Palmer, Prentice Hall.
4. Enzyme Chemistry: Impact and Applications, Ed. Collin J Suckling, Chapman and Hail.
5. Enzyme Mechanisms Ed, M. 1. Page and A. Williams, Royal Society of Chemistry.
6. Enzymatic Reaction Mechanisms, C. Walsh, W. H. Freeman.
7. Enzyme Structure and Mechanism, A Fersht, W.H. Freeman.
8. Biochemistry: The Chemical Reactions of Living Cells, D. E. MeUler, Academic Press.
9. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
10. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
11. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.

**OR**

## Inorganic Photochemistry [Course Code : 1Y2CHE201]

**Full Marks: 50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Excited States of Metal Complexes** **10 Hrs**

Excited states of metal complexes: comparison with organic compounds, electronically excited states of metal complexes, charge-transfer spectra, charge transfer excitations, methods for obtaining charge-transfer spectra.

**II Ligand Field Photochemistry** **10 Hrs**

Photosubstitution, photooxidation and photoreduction, lability and selectivity, zero vibrational levels of ground state and excited state, energy content of excited state, zerozero spectroscopic energy, development of the equations for redox potentials of the excited states.

**III Redox Reactions by Excited Metal Complexes** **20 Hrs**

Energy transfer under conditions of weak interaction and strong interaction-exciplex formation; conditions of the excited states to be useful as redox reactants, excited electron transfer, metal complexes as attractive candidates (2,2'-bipyridine and 1,10phenonthroline complexes), illustration of reducing and oxidising character of $Ruthenium_2^+$ (bipyridal complex, comparision with $Fe(bipy)_3$; role of spin-orbit coupling-life time of these complexes. Application of redox processes of electronically excited states for catalytic purposes, transformation of low energy reactants into high energy products, chemical energy into light.

**IV Metal Complex Sensitizers** **10 Hrs**

Metal complex sensitizer, electron relay, metal colloid system, semiconductor supported metal or oxide systems, Water photolysis, nitrogen fixation and carbon dioxide reduction

**V NQR spectroscopy and X-ray absorption spectroscopy** **10 Hrs**

NQR isotopes, electric field gradients, Nuclear Quadrupole coupling constants. Experimental techniques and applications. Near edge measurements and EXAFS.

**VI Electron diffraction and Neutron diffraction** **10 Hrs**

Electron diffraction : Experimental technique, Wierl equation, Radial-Distribution method. Neutron diffraction : Principle and Theory, advantages and uses.

**Reference Books**

1 Introduction to Inorganic Photochemistry, Arjun Singh Negi, Cyber Tech Publication, New Delhi.

2 Inorganic Photochemistry, Fmiza Hammer, Sarup Book Publishers Pvt. Ltd., New Delhi.
3. Concepts of Inorganic photochemistry, A. W. Adamson and P D Fleischaves Wiley.
4. Elements of Inorganic Photochemistry G. J. Ferranti, Wiley.
5. Progress in Inorganic Chemistry, Vols 18 and 38 ed. J.J. Lippard, Wiley.

## OR,

## Physical Organic Chemistry [Course Code : 1Y2CHE201]

**Full Marks: 50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Reaction Mechanism: Structure and Reactivity 10 Hrs**

Types of mechanisms, types of reactions, thermodynamic and kinetic requirements, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle. Potential energy diagrams, Transition states and intermediates, methods of determining mechanisms. Theory of isotope effects: Primary and secondary kinetic isotope effects. Heavy atom isotope effects. Tunneling effect. Solvent isotope effects. Effect of structure on reactivity resonance and field effects, Steric effect, quantitative treatment, The transition state theory of isotope effects.

**II Concepts in Molecular Orbital Theory 10 Hrs**

Introduction to Huckel molecular orbital (MO) method as a means to explain modern theoretical methods. Qualitative MO theory - Ionisation potential, Electron denisity. MO energy levels. Orbital symmetry. Orbital interaction diagrams. Huckel theory of conjugated systems: Applications to ethylene, propeny system, cyclopropenyl system, butadiene and cyclobutadiene, bond order and charge density calculations.

**III Steric and Conformational Properties 15 Hrs**

Various type of steric strain and their influence on reactivity. Steric acceleration. Molecular measurements of steric effects upon rates. Steric LFER. Conformational barrier to bond rotation - spectroscopic detection of individual conformers. Acyclic and monocyclic systems. Rotation around partial double bonds. Winstein-Holness and Curtin-Hammett principle.

**IV Structural Effects on Reactivity 15 Hrs**

Linear free energy relationships (LFER). The Hammett equation, Substituent constants, Theories of substituent effects. Taft model, $\sigma_{meta}$- and $\sigma_{para}$-, $\sigma^{+}$ and $\sigma^{-}$ constants, Polar and Steric substituent constants in aliphatic systems, Dual-parameter substituent constant,

**V Principles of Reactivity 20 Hrs**

Mechanistic significance of entropy, enthalpy and Gibb's free energy, solvent polarity scales. Kinetics and Mechanism : The rate equations, first order kinetics through constant concentration of a reagent, kinetic and thermodynamic control, complex systems, The Arrhenius equation, Transition state theory, potential energy surface, The reaction coordinate, Hammond's postulate and its experimental support, Three dimensional reaction coordinate diagrams, Valence bond model, Marcus reaction rate theory, Bell-Evans-Polanyi principle. Potential energy surface model. Electron transfer reactions and theories. Reactivity and selectivity principles.

**Reference Books**


1. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. L. Salem and W. L. Jorgensen,Academic Press.
3. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C.Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular Modeling, W. B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
6. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.


## OR,

## Statistical Thermodynamics and Surface Chemistry

## [Course Code : 1Y2CHE201]

**Full Marks: 50+20+30**

**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Statistical Thermodynamics** **15 Hrs**

Concept of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging, Canonical, grand canonical and microcanonical ensembles, corresponding distribution laws (using Lagrange's method of undetermined multipliers). Partition functions-translational, rotational, vibrational and electronic partition functions. Applications of partition functions, Fermi-Dirac statistics, distribution law and applications to metal. Bose-Einstein statistics. Distribution law and its application to helium.

**II Potential Energy Surfaces** **10 Hrs**

Mechanism of activation, Potential energy surface for three atom reaction, Potential energy curve for successive reations, Properties of potential energy surfaces, Inter conversion of translational and vibrational energies, Combination of atoms, Ortho-para conversion, Activated state of three atom and four atom reactions, Potential energy profile, reaction co-ordinate, Transmission co-efficient, non-adiabatic reaction.

**III Kinetics of condensed phase reactions** **10 Hrs**

Rate determining steps in diffusion controlled reactions and activation controlled reactions, Stokes-Einstein equation and dependence of rate constant on co-efficient of viscosity of medium, Kinetics of ionic reactions in solution-electrostatic contribution to free energy in single and double spherical models of activated complex, entropy of activation for ion-ion reactions; Kinetics of dipole-dipole reaction, ion-dipole reaction, dependence of rate constant on ionic strength and dielectric constant of medium, Bronsted-Bjerrum equation.

**IV Study of Fast Reactions** **10 Hrs**

Photophysical Chemistry - Flash Photolysis, Relaxation technique, Nuclear Magnetic Resonance Method, Molecular Beam and Shock-tube Kinetics, Flow method. Reactions of Protons, Electrons metal ions.

**V Surface Chemistry** **25 Hrs**

**A. Adsorption :** Surface tension, capillary action, pressure difference across curved surface (Laplace equation), Vapour pressure of droplets (Kelvin equation), Classical and modern methods for determining surface structure and composition, Surface films on liquids (Electro-kinetic phenomena), criteria for spreading of one liquid on another, Surface pressure and measurement of surface pressure, Langmuir surface balance and

molecular dimensions, states of mononuclear films, reaction in monomolecular films , types and structure of surface films: optical method, electrical method.

**B. Micelles :** Surface active agents, classification of surface active agents, micellization, hydrophobic interaction, critical micellar concentration (CIVIC), factors affecting the CIVIC of surfactants, counter ion binding to micelles, thermodynamics micellization-phase separation and mass action models, solubilization, micro emulsion, reverse micelles.

**C. Macromolecules :** Polymer-definition, types of polymers, electrically conducting, fire resistant, liquid crystal polymers, kinetics of polymerization, mechanism of polymerization.

Molecular mass, number and mass average molecular mass, molecular mass determination (osmometry, viscometry, diffusion and light scattering methods), sedimentation, chain configuration of macromolecules, calculation of average dimensions of various chain structures.

**Reference Books**


1. Physical Chemistry- Waller J. Moore
2. Physical Chemistry - P.W. Atkins, ELBS.
3. Principles of polymer chemistry Cornell , P. J. Flory (Univ. Press)
4. Handbook of Conducting Polymers Vol I & II" T A. Skolhia.
5. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
6. Quantum Chemistry, Ira N. Levine, Prentice Hall.
7. Coulson's Valence, R. McWeeny, ELBS.
8. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
9. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.
10. Modern Electrochemistry Vol. I and Vol. II, J.O.M. Bockris and A.K.N. Reddy, Plenum.
11. Introduction to Polymer Science, V.R. Gowarikar, N.V. Vishwanathan and J. Sridhar, Wiley Eastern.

# M.Sc. Semester-II
# Core Course – 4 (CC-4)
# Course Code : 1Y2CHE202
## (Quantum Chemistry and Chemical Dynamics)

**Full Marks:**
**50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

## I. Quantum Chemistry 35 Hrs

A. Introduction to Exact Quantum Mechanical Results

Concept of operator, The Schrodinger equation and the postulates of quantum mechanics. Discussion of solutions of the Schrodinger equation to some model systems viz., particle in a box, the harmonic oscillator, the rigid rotor, the hydrogen atom. B. Approximate Methods

The variation theorem, linear variation principle. Perturbation theory (first order and non-degenerate). Applications of variation method and perturbation theory to the Hydrgen atom.

C. Qualitative treatment of hydrogen atom

Setting up of Schrödinger equation in spherical polar coordinates, radial part, quantization of energy (only final energy expression).

D. Chemical bonding

Covalent bonding, valence bond and molecular orbital approaches, LCAO-MO treatment of $H_2^+$. Bonding and antibonding orbitals. Qualitative extension to $H_2$. Comparison of LCAO-MO and VB treatments of $H_2$ (only wavefunctions, detailed solution not required) and their limitations. Refinements of the two approaches (Configuration Interaction for MO, ionic terms in VB). Qualitative description of LCAO-MO treatment of homonuclear and heteronuclear diatomic molecules (HF, LiH). Localised and non-localised molecular orbitals treatment of triatomic ($BeH_2$, $H_2O$) molecules. Qualitative MO theory and its application to $AH_2$ type molecules.

E. Angular Momentum

Ordinary angular momentum, generalized angular momentum, eigen-functions for angular momentum, eigen-values of angular momentum, operator using ladder operators, addition of angular momenta, spin, antisymmetry and Pauli exclusion principle.

F. Electronic Structure of Atoms

Electronic configuration, Russell-Saunders terms and coupling schemes, Slater-Condon parameters, term separation energies of the $p^n$ configuration, term separation energies for the $d^n$-configurations, magnetic effects: spin-orbit coupling and Zeeman splitting, introduction to the methods of self-consistent field, the virial theorem.

## II Classical Thermodynamics 15 Hrs

Brief resume of concepts of laws of thermodynamics, free energy, chemical potential and entropies.Partial molar properties; partial molar free energy, partial molar volume and partial molar heat content and their significances. Determinations of these quantities. Concept of fugacity and determination of fugacity. Non-ideal systems: Excess functions for non-ideal solutions. Activity, activity coefficient, Debye-Huckel theory for activity coefficient of electrolytic solutions; determination of activity and activity coefficients; ionic

strength. Gibb's Duhen equation, Nernst heat theorem and its applications, Determination of ablolute entropy, Maxwell's thermodynamic relation.

**III Chemical Dynamics** **20 Hrs**

Methods of determining rate laws, collision theory of reaction rates, steric factor, activated complex theory, Arrhenius equation and the activated complex theory; ionic reactions, kinetic salt effects, steady state kinetics, kinetic and thermodynamic control of reactions, treatment of unimolecular reactions.

Dynamic chain (hydrogen-bromine reaction, pyrolysis of acetaldehyde, decomposition of ethane), photochemical (hydrogen-bromine and hydrogen-chlorine reactions) and oscillatory reactions (Belousov -Zhabotinsky reaction), homogeneous catalysis, kinetics of enzyme reactions, general features of fast reactions, study of fast reactions by flow method, relaxation method, flash photolysis and the nuclear magnetic resonance method. Dynamics of molecular motions, probing the transition state, dynamics of barrierless chemical reactions in solution, dynamics of unimolecular reactions (Lindemann - Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRKM] theories of unimolecular reactions).

**Reference Books**


1. Physical Chemistry, P.W. Atkins, ELBS.
2. Introduction to Quantum Chemistry, A.K. Chandra, Tata McGraw Hill.
3. Quantum Chemistry, Ira N. Levine, Prentice Hall.
4. Coulson's Valence, R. McWeeny, ELBS.
5. Chemical Kinetics, K. J. Laidler, Mcgraw-Hill.
6. Kinetics and Mechanism of Chemical Transformations, J. Rajaraman and J. Kuriacose, McMillan.

# M.Sc. Semester-II
# Core Course – 5 (CC-5)
# Course Code : 1Y2CHE203
## (Group Theory and Spectroscopy)

**Full Marks:**
**50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Symmetry and Group Theory in Chemistry** **25 Hrs**

Symmetry elements and symmetry operation, Group and Subgroup, Point group, Classification and representation of groups, The defining property of a group, Sub group and Class, Group multiplication table for $C_{2v}$, $C_{2h}$ and $C_{3v}$ point group, Generators and Cyclic groups. Similarity Transformation, Table of conjugates for $C_{2v}$, $C_{2h}$ and $C_{3v}$ point group, Schonflies symbols.

Matrix notation for symmetry operation, Representations of groups by matrices (representation for the Cn, Cnv, Cnh and Dnh groups to be worked out explicitly). Character of a representation, Mulliken symbols for irreducible representations, Direct product relationship, Applications of group theory to quantum mechanics-identifying non-zero matrix elements.

The great orthogonal theorem (without proof) and rules derived from this theorem. Derivation of the orthonormalization condition. Character table. Construction of character table: $C_{2v}$ and $C_{3v}$ (only). Reducible representations and their reduction. Application of character table in determination of IR and Raman active vibrations in $H_2O$, $BF_3$ and $N_2F_2$.

**II Microwave Spectroscopy** **10 Hrs**

Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor. Stark effect, nuclear and electron spin interaction and effect of external field.

**III Vibrational Spectroscopy** **15 Hrs**

**A. Infrared Spectroscopy**

Review of linear harmonic oscillator, vibrational energies of diatomic molecules, zero point energy, force constant and bond strengths; anharmonicity, Morse potential energy diagram, vibration-rotation spectroscopy, P,Q,R branches. Breakdown of Oppenheimer approximation; vibrations of polyatomic molecules. Selection rules, normal modes of vibration, group frequencies, overtones, hot bands, factors affecting the band positions and intensities, far IR region, metal-ligand vibrations, normal co-ordinate analysis,

**B. Raman Spectroscopy**

Classical and quantum theories of Raman effect. Pure rotational, vibrational and vibrational-rotational Raman spectra, selection rules, mutual exclusion principle. Resonance Raman spectroscopy, coherent anti Stokes Raman spectroscopy (CARS).

**IV Electronic Spectroscopy** **10 Hrs**

**A. Atomic Spectroscopy**

Energies of atomic orbitals, vector representation of momenta and vector coupling, spectra of hydrogen atom and alkali metal atoms.

**B. Molecular Spectroscopy**

Energy levels, molecular orbitals, vibronic transitions, vibrational progressions and geometry of the excited states, Franck-Condon principle, electronic spectra of polyatomic molecules. Emission spectra; radiative and non-radiative decay, internal conversion, spectra of transition metal complexes, charge-transfer spectra.

**V Mass Spectrometry** **10 Hrs**

Basic principles - Ion production : Soft ionization methods, Low energy electron ejection, Chemical ionization, Ionization of large molecules : Fast-atom bombardment (FAB), Plasma desorption (PD) and Matrix Assisted Laser Desorption/ionization (MALDI), Electrospray ionization (ESI), Pyrolysis, Exact mass measurements, Tandem mass spectrometry. Quadrapole mass spectrometers: FT-ICR

**Reference Books**


1. F. A. Cotton, Chemical Application of Group Theory , John wiley and Sons Inc.,Newyork, 1971.
2. N. Tinkham, Group Theory and Quantum Mechanics , McGraw Hill Book Company, Newyork, 1964.
3. Alan Vincent, Molecular Symmetry and Group theory – Programmed Introduction to chemical applications , Wiley, Newyork, 1977.
4. Physical Methods for Chemistry, R.S. Drago, Saunders Company.
5. Modern Spectroscopy, J.M. Hollas, John Wiley.
6. Physical Methods in Chemistry, R.S. Drago, Saunders College.
7. Introduction to Molecular Spectroscopy, Q.M. Barrow, McCraw Hill.
8. Basic Principles of Spectroscopy. R. Chang, McGraw Hill.
9. Theory and Applications of UV Spectroscopy, H.H. Jatie and M. Orehin, IBH-Oxford.
10. Introduction to Magnetic Resonance, A. Carrington and A.D. Maclachalan, Harper & Row.
11. Structural Methods in Inorganic Chemistry, E.A.V. Ebsworth, D.W.H. Rankin and S. Cradock, ELBS
12. Infrared and Raman Spectra: Inorganic and Coordination Compounds, K. Nakamoto, Wiley.
13. NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry, R.V. Parish, Ellis Horwood.
14. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age Publications.
15. Introduction to Molecular Spectroscopy, C. N. Banwell, TMH Edition.

# M.Sc. Semester-II
# Core Corse (P) – 6 [CC(P)-6]
# Course Code : 1Y2CHE204P
## Physical Chemistry

**Full Marks: 100**
**Pass Marks: 34**
**Time: 06 Hrs**

Two questions are to be set.

**1. Measurement of density of gases and vapours**
- (a) Victor Meyer's Method Determination of Molecular weight of Acetone, Chloroform, Benzene, (Mixture).
- (b) Duma's Method Determination of molecular weight of acetone, Carbon-Tetrachloride.

**2. Determination of Molecular weight of substances**
- (a) Beckmann's freezing point Method
- (b) Beckmann's Boiling point method.

**3. Viscosity of liquids and solution by Ostwald tube**
Determination of percentage composition of a mixture of two liquids.

**4. Surface Tension of liquids and solutions**
- (a) Study of the effect of conc. on surface tension of acetic acid and Sod. Chloride solutions.
- (b) Determination of Parachor.

**5. Thermochemistry**
- (a) Determination of water equivalent of a calorimeter
- (b) Determination of the Heat of Neutralization of :
  - (i) Strong acid and strong base (HCl and NaOH)
  - (ii) Weak acid and strong base (NaOH and $CH_3$ COOH).
- (c) Determination of Heat of solution of Potassium Nitrate
- (d) Determination of basicity of succinic Acid by Thermochemical Method.

**6. Order of Reaction**
- (a) Determination of the rate constant of hydrolysis of an ester with an acid (Methyl acetate and HCl).
- (b) Determination of the rate constant of saponification of ethyl acetate by NaOH.

**7. Partition Co-efficient**
  - (i) Benzoic acid between water and Benzene
  - (ii) Iodine between water and carbon tetrachloride

**8.** Estimation of following in the supplied water,
Ca, Iron, Lead, Mg, Nitrate, Chloride

**9.** Estimation of following in the supplied soil sample,
Ca, Mg, Carbonate carbon, Organic matter, Total nitrogen, Ammonia, Nitrate nitrogen

**Practical-1: 50 Marks, Note Book: 20 Marks, Viva: 30 Marks.**

| COURSE STRUCTURE OF M.Sc CHEMISTRY THIRD SEMESTER | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Course Details | | | | External Assessment | | Internal Assessment | | | | Credit Distribution | | | Allotted Credits |
| Course Code | Course Type | Course Title | Total Marks | Major | | Minor | | Sessional | | L | T | P | Subjectwise Distribution |
| | | | | Max. Marks | Min. Marks | Max. Marks | Min. Marks | Max. Marks | Min. Marks | | | | |
| 1Y2CHE301 | Core Course - VII | Application of Spectroscopy | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE302 | Core Course -VIII | Environmental Chemistry | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE303 | Elective Course -II | Elective Course | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE304P | Elective Course - Practical-3 | Elective Course Practical | 100 | 50 | 17 | 20 | 07 | 30 | 10 | - | - | 10 | 5 |
| | Grand Total | | 400 | | | | | | | | | | 20 |

**Minimum Passing Marks are equivalent to Grade D**
**Lectures T- Tutorials P- Practical, Major- Term End Theory Exam**
**Minor- Pre University Test**
**Sessional weightage – Attendance 50%, Three Class Tests/Assignments 50%**

# M.Sc. Semester-III
# Core Course – 7 (CC-7)
# Course Code : 1Y2CHE301
## Application of Spectroscopy

**Full Marks:**
**50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Ultraviolet and Visible Spectroscopy** **10 Hrs**

Types of electronic transitions (185-800 nm), Beer-Lambert law, Effect of solvent polarity on electronic transitions, Chromophores and Auxochromes, Absorption and Intensity shift; Bathochromic, Hypsochromic shifts, Hyperchromic and Hypochromic shifts. Application of Fieser-Woodward Rules for calculation of $\lambda_{max}$ for Conjugated dienes: alicyclic, homoannular, heteroannular, extended conjugated systems (aldehydes, ketones and dienes), Distinction between cis and trans isomers. Application of Fieser-Woodward Rules for calculation of $\lambda_{max}$ for the following systems: α, β - unsaturated aldehydes, ketones, carboxylic acids and esters. Ultraviolet and visible spectra of aromatic and heterocyclic compounds.

**II Infrared Spectoscopy** **10 Hrs**

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

**III Nuclear Magnetic Resonance Spectroscopy** **15 Hrs**

Basic principle of PMR Spectroscopy, chemical shift, spin-spin coupling and coupling constant, Pascal's triangle-low and high resolution, reference compounds (internal and external), nuclear shielding and deshielding phenomenon, chemical shift and factors influencing it, Anisotropic effects in alkene, alkyne, aldehydes, acids and aromatics. Chemical shift correlation for protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic) and other nuclei (alcohols, phenols, enols, carboxylic acids, amines and amides), chemical exchange, effect of deuteration, solvent effects. Fourier transform technique.

Interpretation of PMR spectra of simple organic compounds (such as ethyl bromide, ethanol, 1,1,2-tribromoethane, acetaldehyde, acetic acid and ethyl acetate).

**$^{13}$C-NMR Spectroscopy** **05 Hrs**

General considerations, chemical shift (aliphatic, olefinic, alkyne, aromatic, heteroaromatic and carbonyi carbon), coupling constants. Two dimension NMR spectroscopy - COSY, NOESY, DEPT, INEPT, APT and INADEQUATE techniques.

**IV Mass Spectrometry** **10 Hrs**

Introduction, ion production - El, Cl, FD and FAB, factors affecting fragmentation, ion

analysis, ion abundance. Mass spectral fragmentation of organic compounds : alkanes, alkenes, alkyl halides, alcohols, aldehydes, ketones (cyclic and acyclic compounds), acids, esters, ethers, amines, nitro compounds, halo compounds and peptides. Factors affecting cleavage patterns. Molecular ion peak, Metastable peak, McLafferty rearrangement. Nitrogen rule. High resolution mass spectrometery. Examples of mass spectral fragmentation of organic compounds with respect to their structure determination. Use of HRMS to determine exact molecular weight of compounds

**V Electron Spin Resonance Spectroscopy** **10 Hrs**

Hyperfine coupling, spin polarization for atoms and transition metal ions, spin-orbit coupling and significance of g-tensors, application to transition metal complexes (having one to five unpaired electrons) including biological systems and to inorganic free radicals such as $PH_4$, $F_2^-$ and $[BH_3]^-$.

**VI Mössbauer Spectroscopy** **10 Hrs**

Basic principles, Isomer shift, Quadrupole splitting and Magnetic hyperfine interactions. Application of the technique to the studies of (1) bonding and structures of $Fe^{+2}$ and $Fe^{+3}$ compounds including those of intermediate spin, (2) $Sn^{+2}$ and $Sn^{+4}$ compounds, nature of M-L bond, coordination number, structure and (3) detection of oxidation state and inequivalent MB atoms.

**Reference Books**


1. Organic Spectroscopy, P. Laszlo and P. Strang, Harper and Row, New York, 1971.
2. Organic Spectroscopy, W. Kemp, ELBS London, 2000.
3. Introduction to Spectroscopy, 3rd Edition, D. L. Pavia, G. M. Laupman and G. S. Kriz, Harcourt college publishers.
4. Interpretation of Mass Spectra, 4th edition, F.W. McLafferty, F. Turecek, California
5. Practical Organic Mass Spectroscopy, 2nd edition, J. R. Chapman, John Wiley, NY, 1993,
6. The IR spectra of complex molecules, Vols.1 and 2, L. J. Bellamy, Chapman and Hall, London
7. Spectroscopic Techniques for Organic Chemists, J. W. Cooper, John Wiley, NY
8. Bimolecular NMR Spectroscopy, J N S Evans, Oxford univ. 1995.
9. Mass Spectroscopy A Foundation Course. K. Downard, RSC, Cambridge.
10. Instrumental Methods of Analysis, H. H. Willard, L. L. Merrit, J. A. Dean and F.A.Settle, CBS Publishers and Distributors
11. Practical NMR Spectroscopy, M.L Martin, J.J. Delpeuch and Q.J.F Artin, Heyden.
12. Spectrometric Identification of Organic Compounds, R. M. Silverstein, Q. C. gassier and T. C. Morrill, John Wiley
13. Application of Spectroscopy of Organic Compounds, J. R. Dyer, Prentice Hail.
14. Spectroscopic Methods in Organic Chemistry, D. H. Williams, I. Fleming, Tala McGraw Hill.
15. Vibrational Spectroscopy: Theory and Applications, D. N. Sathyanarayana, New Age Publications.

# M.Sc. Semester-III
# Core Course – 8 (CC-8)
# Course Code : 1Y2CHE303
## Environmental Chemistry

**Full Marks:**
**50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Environment and Atmosphere** **10 Hrs**

Introduction.Composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere. Biogeochemical cycles of C, N, P, S and O. Biodistribution of elements. Chemical composition of atmosphere - particles, ions and radicals and their formation. Chemical and photochemical reactions in atmosphere, smog formation, oxides of N, C, S, O, and their effect, pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry. Analytical methods for measuring air pollutants. Continuous monitoring instruments.

**II Hydrosphere** **10 Hrs**

Chemical composition of water bodies-lakes, streams, rivers and wet lands etc. Hydrological cycle. Aquatic pollution - inorganic, organic, pesticide, agricultural, industrial and sewage, detergents, oil spills and oil pollutants. Water quality parameters-dissolved oxygen, biochemical oxygen demand, solids, metals, content of chloride, sulphate, phosphate, nitrate and micro-organisms. Water quality standards. Analytical methods for measuring BOO, DO, COD, F, Oils, metals (As, Cd, Cr, Hg, Pb, Se etc.), residual chloride and chloine demand. Purification and treatment of water.

**III Soils** **05 Hrs**

Composition, micro and macro nutrients, Pollutants-fertilizers, pesticides, plastics and metals. Waste treatment.

**IV Industrial Pollution** **05 Hrs**

Cement, sugar, distillery, drug, paper and pulp, thermal power plants, nuclear power plants, metallurgy. Polymers, drugs etc. Radionuclide analysis. Disposal of wastes and their management.

**V Environmental Toxicology** **10 Hrs**

Chemical solutions to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three rnile island, Sewozo and Minamata disasters.

**VI Analysis of Water Pollution** **10 Hrs**

Origin of waste water, types, water pollutants and their effects. Sources of water pollution-domestic, industrial, agricultural soil and radioactive wastes as sources of pollution. Objectives of analysis-parameter for analysis - colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen. Heavy metal pollution-public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurements of DO, BOD and COD. Pesticides as water pollutants.

**VII Analysis of Soil, Food, Fuel, Body Fluids and Drugs** **20 Hrs**

(a) Analysis of soil: moisture, $p^H$, total nitrogen, phosphorus, silica, lime, magnesia, manganese, sulphur and alkali salts.

(b) Food Analysis: Moisture, ash, crude protein, fat, crude fiber, carbohydrates, calcium, potassium, sodium and phosphate. Food adulteration-common adulterants in food, contamination of food stuffs. Microscopic examination of foods for adulterants. Pesticide analysis in food products. Extraction and purification of sample. HPLC. Gas chromatography for organophosphates. Thin-layer chromatography for identification of chlorinated pesticides in food products.

(c) Fuel analysis: solid, liquid and gas. Ultimate and proximate analysis-heating values - grading of coal. Liquid fuels-flash point, aniline point, octane number and carbon residue. Gaseous fuels-producer gas and water gas-calorific value.

(d) Clinical chemistry: Composition of blood-collection and preservation of samples. Clinical analysis. Serum electrolytes, blood glucose, blood urea nitrogen, uric acid, albumin, globulins, barbiturates, acid and alkaline phosphatases. Immunoassay: principles of radio immunoassay (RIA) and applications. The blood gas analysis of trace elements in the body.

(e) Drug analysis: Narcotics and dangerous drugs. Classification of drugs. Screening by gas and thin-layer chromatography and spectrophotometric measurements.

**Reference Books**


1. Environmental Chemistry, S. E. Manahan, Lewis Publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna Pubilshers.
3. Environmental Chemistry, A. K. De, Wiley Easlem.
4. Environmental Pollution Analysis, S.M. Khopkar, Wiley Eastern
5. Environmental Toxicology, Ed. J. Rose, Gordon and Breach Science Publication.
6. Elemental Analysis of Airborne Particles, Ed. S. Landsberger and M. Crealchman, Gordon and Breach Science Publication.
7. Environmental Chemistry, C. Baird, W. H. Freeman.
8. Handbook of Instrumental Techniques for Analytical Chemistry, F. Settle, Prentice Hall.
9. Fundamentals of Analytical Chemistry, D.A. Skoog, D.M. West and F.J. Holler, W. B. Saunders.

# M.Sc. Semester-III
# Elective (GE/DC) (EC-2)
# Inorganic Chemistry
# Course Code : 1Y2CHE303
**(Organometallic Chemistry)**

**Full Marks: 50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

## I Organotransition Metal Complexes — 15 Hrs

Chemistry of Organotransition metal complexes: General introduction. 18- and 16-Electron rules. General rules. Complexation and De-complexation Reactions: s-Bonded systems including $\eta^1$ ligands. p-Bonded systems involving dihapto to octahapto ligands such as- olefins, acetylenes, allyl moieties, butadiene, cyclobutadiene, arenes, cyclopenta, cyclohexa and cycloheptadienyl moieties; cyclohepta, cyclooctatrienes, and cyclooctatetraene moieties.

Use of organotransition metal complexes as protecting and stabilizing groups: Protection of olefins, acetylenes and dienes. Stabilization of cyclobutadines and norbornadienones. Organometallics as electrophiles and nucleophiles: Nucleophilic addition to $\eta^2$, $\eta^5$ and $\eta^6$ complexes. Electrophilic addition to $\eta^4$, $\eta^6$ and carbene complexes.

## II Organometallic Compounds in Synthesis-II — 15 Hrs

Organometallics in coupling and cyclization reactions: Coupling and cyclization of organic nucleophiles with olefins (including Heck reaction), and coupling of olefins with acetylenes (including Felkin's reaction).

Organometallics in isomerization, oxidation and reduction reactions: Isomerization of olefins, allylic alcohols and allylic ethers. Oxidation of olefins (including Wacker's process and epoxidation) and reduction of olefins and α,β-unsaturated compounds (including Wilkinson's reaction).

## III Organometallic Compounds in Synthesis-III — 30 Hrs

(Organozincs, Organolithiums, Organocopper, Organoseleniums, Organotelluriums, Organoaluminiums, Use of zirconium, iron, cobalt and palladium complexes.)

Application of the following organometallics in synthesis: Organozincs: Preparation, reaction with compounds containing acidic protons, reaction with C-C multiple bonds, trans-metallation, addition reactions of zinc reagents with carbonyl compounds. Organolithiums: Preparation. Deprotonation reactions, nucleophilic addition reactions, reactions with imines, nitriles and isonitriles. Organocopper reagents: (Gilman reagents-lithium dialkyl cuprates): Preparation, reactions with alkyl, allyl, vinyl, benzyl and aryl halides, aldehydes, ketones (including α,β-unsaturated carbonyl compounds) and epoxides.

Organoseleniums: Preparation, use of organoseleniums in the synthesis of alkenes, α,β-unsaturated carbonyl compounds. Organotelluriums: Debromination of vic-dibromides, deoxygenation of epoxides, oxidation of hydroquinone and synthesis of biaryls. Organoaluminiums: Preparation, hydroalumination and carboalumination of alkenes.

Nucleophillic addition reactions with carbonyl compounds and Hydrocyanation. Preparation of alkenyldialkylalanes and their reactions.

Carbonylation reactions: Use of zirconium complexes in the synthesis of esters, acids, aldehydes, acyl halides and in the hydroformylation of olefins and dienes. Use of iron complexes for the insertion of CO group. Use of cobalt complexes in the synthesis of ketones from epoxides, lactones from allylic alcohols and in the hydroformylation of olefins. Use of palladium complexes for the carbonylation of alkyl halides, dienes and allenes.

**IV Organometallic compounds in synthesis-IV** **10 Hrs**

(Organosilicons, Organotins, Organocerates, and Organomercurials)

Organosilicons: Introduction, preparation and general reactions of trialkylsilyl halides. Peterson olefination. Organotins: Preparation and reactions of tri-n-butyltin hydride, Barton decarboxylation and Barton-McCombie reaction. Organocerates: Preparation and reactions of organocerates. Organomercurials: Preparation. Electrophilic substitution reactions. Solvomercuration-demercuration and cyclopropanation of alkenes.

**Reference Books**


1. The Organometallic Chemistry of the transition metals, R. H. Crabtree, 1988.
2. Principles and application of the organotrnsition metal chemistry, J. P. Collman, L. S. Hegedus, University Science books, 1980.
3. Modern Synthetic Reactions, H. O. House, W.A. Benjamin, California, 2nd Edn. 1972.
4. Organometallics, Vol. 1 & 2, M. Bochmann, Oxford Chemistry primers, Oxford University Press, 1994.
5. Organotransition metal chemistry, S. G. Davies, Pergamon Press, Oxford, 1982.
6. Principles and Application of Organotransition Metal Chemistry, J.P. Collman, L.S. Hegsdus, J.R. Norton and R.G. Pinke, University Science Books.
7. The Organometaltic Chemistry o1 the Transition Metals, R.H. Crabtree, John Wiley
8. Metallo-organic Chemistry, A.J. Pearson, Wiley.
9. Organometallic Chemistry, R.C. Mehrotra and A. Singh, New Age International.

**OR,**

# M.Sc. Semester-III
# Elective (GE/DC) (EC-2)
# Course Code : 1Y2CHE303
# Organic Chemistry
## (Supramolecular Chemistry)

**Full Marks: 50+20+30**

**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Supramolecular Chemistry** **20 Hrs**

Bonds weaker than covalent: Ion-ion interaction, ion-dipole interaction, dipole-dipole interaction, Ionic bond, Covalent bond, Hydrogen bonding. Molecular recognition: Molecular receptors for different types of molecules substrates, Supramolecular reactivity and catalysis. Supramolecular devices : Oxa-Crown Ethers, Aza -Crown Ethers, Cryptands, Corands, Podands, Spherands and Hemispherands, C yclophanes, Calixarenes, Cyclodextrines, Catananes, Rotaxanes. Supramolecular reactivity and catalysis: Supramolecules with chiral framework (introduction only), Generating molecular cleft for binding. Some example of self-assembly in supramolecular chemistry, Nanomaterials with supramolecular structure, Molecular devices: Photo-switchable devices.

**II Chemistry of Selected Name Reactions-I** **10 Hrs**

A study of the following name reactions: Dieckmann cyclization, Shapiro reaction, Stork enamine reaction, Barton reaction, Ene reactions, Sharpless asymmetric epoxidation, Bayer–Villiger oxidation, Robinson annulations, Michael addition, Mannich reaction, Simmons-Smith reaction, Hoffmann-Loffler-Freytag reaction, Beker-Venkatraman rearrangement (Few examples in each rearrangement are to be studied).

**III Chemistry of Selected Name Reactions-II** **10 Hrs**

Darzen's reaction, Acid-catalyzed self condensation of olefins, Prins reaction, Hofmann-Martius reaction. Acyloin condensation. Meyer synthesis. Chichibabin reaction, Mitsunobu reaction, N-Nitroaromatic amine rearrangement, Fisher-Hepp reaction. Japp-Klingemann reaction (Few examples in each rearrangement are to be studied).

**IV Rearrangement Reactions** **10 hour**

Formation and stability of carbonium ions, carbanion, carbenes, nitrenes, radicals and arynes. Rearrangement involving carbonium ions: Wagner-Meerwein, Pinacol-Pinacolone rearrangement, reaction involving acyl cation, and Fries rearrangement, Rearrangement involving carbenes: Wolff & Arndst-Eistert synthesis. Rearrangement involving nitrenes: Hoffman, Curtius, Schmidt, Lossen and Beckman rearrangement.

**V Cross Coupling Reactions** **10 Hrs**

The Suzuki-Miyaura reaction, The Heck reaction, Kumada reaction, Nozaki-Hiyama-Kishi reaction and Buchwald-Hartwig reaction.

**VI Biomolecular Spectroscopy** **10 Hrs**

**ORD – CD**: Linearly and circularly polarized light, Circular birefringence and circular dichroism, ORD and CD curves, Cotton effect, Comparison of ORD and CD: Use of plain curves, Application of CD and ORD curves showing Single and Multiple Cotton effects :

(i) Functional group analysis, (ii) Position of a functional group, (ii) Determination of configuration, and (iv) Study of conformational change, Axial haloketone rule, Octant rule for ketones and its application.

**Reference Books**


1. Molecular Mechanics, U. Burkert and N. L. Allinger, ACS Monograph 177, 1982.
2. Organic Chemists' Book of Orbitals. L. Salem and W. L. Jorgensen,Academic Press.
3. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C.Richardson, Harper and Row.
4. Introduction to Theoretical Organic Chemistry and Molecular Modeling, W. B. Smith, VCH, Weinheim.
5. Physical Organic Chemistry, N. S. Isaacs, ELBS/Longman.
6. Supramolecular Chemistry., Concepts and Perspectives, J. M. Lehn, VCH.
7. The Physical Basis of Organic Chemistry, H. Maskill, Oxford University Press.

**OR,**

# M.Sc. Semester-III
# Elective (GE/DC) (EC-2)
# Physical Chemistry
## (Solid State Chemistry)
# Course Code : 1Y2CHE303

**Full Marks: 50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Diffraction Theory and Single Crystal XRD** **20 Hrs**

Symmetry elements, Bravais lattices, Miller indices, Laue method, Screw axes and glide planes, point groups & space groups and nomenclature. Law of Interfacial angle (Euler's construction). X-rays, Bragg's law, assignment of lines, diffraction pattern of a primitive cubic lattice, space group extinctions, Scaterring factor and structure factor, Identification of unit cells from systematic absences in diffraction pattern. Structure of simple lattices and X-ray intensities, Intensities from atomic positions for BCC and FCC lattices, Procedure for an X-ray structure analysis, Ewald's sphere of reflection, Reciprocal Lattice concept, Fourier transform of the structure factor, Phase problem and Patterson synthesis, Absolute configuration of molecules, Ramchandran diagram. Weissenberg and Precession methods. Debye-Scherrer method (Powder method), Determination of lattice parameters from these methods. Experimental technique: Wierl equation, Radial-Distribution method.

**II Superconductivity** **10 Hrs**

Superconductivity, Meissner effect, Type I and type II superconductors, Features of superconductors, Microscopic theory of superconductivity, Frolich diagram, Cooper pairs, Theory of low temperature superconductivity, Conventional organic and high temperature superconductors, Fullerenes, Applications of superconductors. Transformation in crystals - thermodynamics of transformation, Classification of phase transitions, First and second order phase transitions: Order-disorder transitions, Martensitic transition and spinodal decomposition, Polymorphic transformation.

**III Conducting Polymers** **10 Hrs**

Electrically conducting polymers electrochemical polymerization, band structure of polymers, mechanism of conduction in polymers, doping of polymers, application of conduction polymers.

**IV Polymer Liquid Crystal** **10 Hrs**

Polymer liquid crystal, nematic, cholesteric and smectic phases, liquid crystalline order of the main chain and of the side groups in polymers, synthesis and properties of polymer liquid crystals, liquid crystalline order in biological materials.

**V Electronic Structure of Solids** **10 Hrs**

Bonding in solids: Ionic, covalent, metallic and molecular solids, Free electron theory, band theory, Fermi sphere, Fermi-Dirac statistics, limitations of the free electron theory Electrons in a weak periodic potential (Independent electron model), Brillouin zone, wave

function for electrons in solids, metallic conductors, insulator, semiconductors (intrinsic & extrinsic), properties of junctions, energy levels in extended, repeat and reduced zone schemes.

**VI Electrical and Magnetic Properties of Solids** **10 Hrs**

Metals: calculation of density of states, origin of resistivity, weak paramagnetism Semiconductors: Intrinsic and extrinsic- p and n-types, Hall effect, Junctions and their applications: metal-metal, metal-semiconductor, semiconductor-semiconductor types and transistors. Insulators - dielectric properties, piezo and inverse piezoelectric effects, ferroelectricity, ferroelectric transitions in $BaTiO_3$, ionic conductivity applications of band theory to TiO and NiO: Limitations of the Independent electron model, modeling electron correlation.

**Reference Books**


1. Crystallography, Philips
2. Solid State chernistry, Garner (Butterworth; London)
3. Solid State Chemistry, D.K. Chakraborty (New Age int Publication)
4. Solid State Chemistry, N. B. Hannay (Prentice Hall, New Jersay)
5. Physical Chemistry, P.W. Atkins
6. Principles of Polymer Chemistry, P. J. Flory (Univ. Press)
7. Handbook of Conducting Polymers Vol I & II", T A. Skolhia.

# M.Sc. Semester-III

## Inorganic Chemistry Practical

## EC(P)-3

## Course Code : 1Y2CHE304P

**Full Marks: 100**
**Pass Marks: 34**
**Time : 06 Hrs**

Two questions are to be set.

1. Qualitative separation and determination of the following pairs of metal ion using gravimetric and volumetric methods
   a) $Ag^{+}$(g) and $Cu^{2+}$(v)
   b) $Cu^{2+}$(g) and $Zn^{2+}$(v)
   c) $Fe^{3+}$(g) and $Ca^{2+}$ (v)
   d) $Mg^{2+}$(g) and $Ca^{2+}$ (v)
2. Semi micro qualitative analysis of a mixture containing five cations of rare element and insolables.
   a) Rare element Tl, W Sc Mo, Ti, Zr Ce, Tb V, V, Lx
   b) Insoluble $PbSO_4$, $SrSO_4$, $Al_2O_3$ $Cr_2O_3$, $Fe_2O_3$, $SnO_2$, $ThO_2$, $WO_3$

3. Gravimetric Analysis

   a) Estimation of nickel (II) using Dimethylglyoxime (DMG)
   b) Estimation of copper as CuSCN
   c) Estimation of iron as $Fe_2O_3$ by precipitating iron as $Fe(OH)_3$
   d) Estimation of Al (III) by precipitating with oxine and weighing as $Al(oxine)_3$

4. Inorganic Preparations
   a) Cis and trans $K[Cr(C_2O_4)_2.(H_2O)_2]$ Potassium dioxalatodiaquachromate (III)
   b) Tetraamminecarbonatocobalt (III) ion
   c) Potassium tris(oxalate)ferrate(III)
   d) Tetraamminecopper (II) sulphate, $[Cu(NH_3)_4]SO_4.H_2O$

**Practical: 50 Marks, Note Book: 20 Marks, Viva: 30 Marks.**

**OR,**

# M.Sc. Semester-III

## Organic Chemistry Practical

## EC(P)-3

## Course Code : 1Y2CHE304P

**Full Marks: 100**
**Pass Marks: 34**
**Time : 06 Hrs**

Two questions are to be set.

**I Separation and Characterization of organic compounds from Binary systems:**

(i) liquid-liquid,
(ii) liquid-solid
(iii) solid-solid

**II Preparation of organic compounds using methods not involving more than two steps:**

(i) Preparation of o-Chlorobenzoic Acid from Anthranilic acid
(ii) Preparation of Iodobenzene from Aniline
(iv) Preparation of p-Iodonitrobenzene from p-Nitroaniline
(v) Anthraquinone from anthracene
(vi) β-naphthyl methyl ether from β-naphthol

**III Estimation:**

(a) To determine the percentage or number of phenolic groups in the given sample by The acetylation method.
(b) To determine the percentage or number of methoxyl groups in the gtiven sample by The Zeisel's method.
(c) To determine the percentage or number of acetyl groups in an Acetyl Ester

**IV Estimation of the amount of HCHO in the given solution by sodium sulphite method.**

**Practical-1: 50 Marks, Note Book: 20 Marks, Viva: 30 Marks.**

## OR,

## M.Sc. Semester-III

### Physical Chemistry Practical

## EC(P)-3

## Course Code : 1Y2CHE304P

Two questions are to be set.

**Full Marks: 100**
**Pass Marks: 34**
**Time : 06 Hrs**

**I Conductometry**

1. To determine the solubility and solubility product of a sparingly soluble salt
2. To verify Onsager equation for a uni-univalent electrolyte in aqueous solution
3. To titrate a mixture of HCl, $CH_3COOH$ and $CuSO_4$ with NaOH
4. To determine the rate constant of saponification of an ester by NaOH.

**II. Potentiometry**

1. To determine the solubility and solubility product of AgCl in water
2. To determine the $E_0$ of $Zn/Zn^{++}$, $Cu/Cu^{++}$ ELECTRODES.
3. To determine the basicity of a polybasic acid and its dissociation constant.
4. To investigate the complex formed between $CuSO_4$ and $NH_3$.

**III. Polarimetry**

1. To analyse a mixture of glucose and sucrose
2. To study the inversion of cane sugar in acid medium.

**IV. Refractometry**

1. To verify mixture law of refraction
2. To determine the composition of an unknown solution.

**V.Cryoscopy**

1. To determine the activity of a non-electrolyte by freezing point method
2. To determine the mean activity co-efficient of KCl by freezing point method.

**Practical-1: 50 Marks, Note Book: 20 Marks, Viva: 30 Marks.**

| COURSE STRUCTURE OF M.Sc CHEMISTRY FOURTH SEMESTER | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Course Details | | | | External Assessment | | Internal Assessment | | | | Credit Distribution | | | Allotted Credits |
| Course Code | Course Type | Course Title | Total Marks | Major | | Minor | | Sessional | | L | T | P | Subjectwise Distribution |
| | | | | Max. Marks | Min. Marks | Max. Marks | Min. Marks | Max. Marks | Min. Marks | | | | |
| 1Y2CHE401 | Core Course-IX | Synthetic Organic Chemistry | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE402 | Elective Course-IV | Elective Course-IV | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE403P | Elective Course-V Practical | Elective Course-V Practical | 100 | 50 | 17 | 20 | 07 | 30 | 10 | 5 | 1 | - | 5 |
| 1Y2CHE404PR | Project | Project | 100 | - | - | - | - | - | - | - | - | 10 | 5 |
| | Grand Total | | 400 | | | | | | | | | | 20 |

**Minimum Passing Marks are equivalent to Grade D**
**Lectures T- Tutorials P- Practical, Major- Term End Theory Exam**
**Minor- Pre University Test**
**Sessional weightage – Attendance 50%, Three Class Tests/Assignments 50%**

# M.Sc. Semester-IV
# Core Course – 9 (CC-9)
### Synthetic Organic Chemistry
# Course Code : 1Y2CHE401

**Full Marks: 50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

## I Retro-synthesis 10 Hrs

Retro synthetic analysis : Definition, Synthon approach, Synthetic equivalent, Linear and convergent method in organic synthesis, Disconnection approach : One group disconnection, Retro synthesis of alcohols, Retro Diels-Alder reaction, Retro synthesis of olefins, Retro synthesis of aliphatic ketones.

## II Pericyclic Reactions 20 Hrs

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1, 3, 5-hexatriene, allyl system, Classification of pericyclic reactions. FMO approach, Woodward-Hoffman correlation diagram method and PMO approach for pericyclic reaction under thermal and photochemical conditions.

Electrocyclic reactions: Conrotatary and disrotatary motion, 4n and (4n+2) systems, Cycloaddition reaction: [2+2] and [4+2] cycloaddition reaction, Cycloaddition of ketones, Secondary effects in [4+2] cycloaddition. Stereochemical effects on rate of cycloaddition reaction, Diels-Alder reaction, 1,3-dipolar cycloaddition, Chelotropic reaction, The Nazarov reaction.

Sigmotropic rearrangement: Suprafacial and antarafacial shift involving H and carbon-moieties, Peripatetic cyclopropane bridge, Retention and inversion of configuration, [3,3]-, [1,5]-, [2,3]-, [4,5]-, [5,5]-, and [9,9]-Sigmatropic rearrangements, Claisen rearrangements (including Aza-Claisen, Ireland-Claisen), Cope rearrangements (including Oxy-Cope, Aza-Cope), Sommelet-Hauser rearrangements, Group transfer reaction, Ene reaction, Mislow - Evans rearrangement, Walk rearrangement.

## III Photochemistry 10 Hrs

Thermal versus photochemical reactions, Electronic excitations: n–π* and π–π* transitions. Singlet and Triplet energy states: Comparison of energies, Lifetimes and Reactivity. Jablonski diagram, Allowed and forbidden transitions: Fluorescence, Phosphorescence, Internal conversion and Intersystem crossing.

Photochemical reactions of saturated ketones : Norrish Type I and Norrish Type II reaction, Photoreduction of ketone, Photoaddition reactions, Paterno-Buchi reaction. Photochemistry of simple olefins : Cis-trans isomerization, Di-pi methane rearrangement. Photooxidation : Formation of peroxy compounds, oxidative couplings : Barton reaction. Photo rearrangements : Photo-Fries rearrangement and Photo rearrangement of 2,5-Cyclohexadienones.

**IV Reagents in Oxidation Reactions** **15 Hrs**

DDQ, Oxidation with $SeO_2$, Epoxidation of olefins, Sharpless asymmetric epoxidation, Robinson annulations, Dihydroxylation of olefins using $KMnO_4$ and $OsO_4$, Woodward and Prevost dihydroxylation, Oxidative cleavage of olefins, Ozonolysis, (i) Oxidation of alcohols: Chromium reagents, Pyridinium chlorochromate (PCC), Collin and Jones reagent, DCC, Oxidation with $MnO_2$, Oppenauer oxidation. (i) Oxidation of aldehydes and ketones: Baeyer-Villiger oxidation, $Pb(OAc)_4$, Dess-Martin periiodinane. (With stereochemistry of oxidation).

**V Reagents in Reduction Reactions** **15 Hrs**

Catalytic hydrogenation: Raney Ni-catalyst, Adam catalyst, Lindlar catalyst, Wilkinson catalyst. (ii) Reduction by dissolving metals: Birch reduction, Hydrogenolysis (iii) Reduction by hydride transfer reagents: MPV reduction, Reduction with $LiAlH_4$ and $NaBH_4$, Diisobutylaluminium hydride (DIBAL-H), Reduction with boranes and derivatives, Reduction with $Bu_3SnH$, Reduction of carbonyl group to methylene, Reduction with trialkylsilanes. (With stereochemistry of reduction).

**Reference Books**


1. Jerry March, Advanced Organic Chemistry -Reactions, Mechanisms and Structure , Fourth Edition, John Wiley & Sons (1992)
2. P.S. Kalsi, Organic Reactions and Mechanisms , Second Edition, New Age International Publishers, 2002.
3. P.S. Kalsi, Stereochemistry – Conformation and Mechanism , 6 th Edition, Wiley Eastern Limited, 2005.
4. I.L. Finar, Organic Chemistry , Volume II, Fifth Edition, First Indian reprint, Pearson Education Asia Pte. Ltd., (2000)
5. S.M. Mukherji and S. P. Singh, Reaction Mechanism in Organic Chemistry , 1 st Edition, Macmillan, 1976.
6. R.T. Morrison and R.N. Boyd, Organic Chemistry , Prentice-Hall, 1992.
7. R.O.C. Norman, Principles of Organic Synthesis , Second Edition, Chapman and Hall, 1978.
8. Fundamentals of Photochemistry, K.K. Rohatgi Mukhergee, Wiley Eastern Limited
9. Photochemistry, Carol E Wayne and Richard P Wayne, Oxford University Press(1996)
10. Organic Photochemistry, J. M. Cozen and B. Halton, Cambridge University Press ($1^{st}$ Edition) 1974
11. Molecular Reactions and Photochemistry, C H Deputy and D S Chapman, Prentice Hall India, New Delhi ( 1st Edition) , 1972.

# M.Sc. Semester-IV
# Elective (GE/DC) [EC-4]
# Inorganic Chemistry
## (Metal Clusters)
## Course Code : 1Y2CHE402

**Full Marks: 50+20+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Metal Clusters, Metal-metal bonding and Metal -Complexes 20 Hrs**

Higher boranes, carboranes, metalloboranes, metallocarboranes and Halide clusters. Polyhedral model of metal clusters, effect of electronic configuration and coordination number. Structures of metal carbonyl clusters of three atoms $M_3(CO)_{12}$ (M=Fe, Ru & Os), Four metal atoms tetrahedra $M_4(CO)_{12}$ [M= Co, Rh & Ir] and octahedron of type $M_6(CO)_{16}$ [M = Co & Rh], and halide derivatives of Rhenium (III) triangles, metal carbonyls involving bridged-terminal exchange and scrambling of CO group. Electron counting in carbonyl clusters, Wades-Mingos and Lauher rules. Vibrational spectra of metal carbonyls for bonding and structure elucidation, Important reactions of metal carbonyls. Preparation, Bonding, Structure and Important reactions of transition metal Nitrosyl, Dinitrogen and Dioxygen complexes. Tertiary phosphine as ligand.

**II Metal-Ligand Bonding and Complex metal hydrides 10 Hrs**

Limitation of crystal field theory, molecular orbital theory, octahedral, tetrahedral and square planar complexes, p-bonding and molecular orbital theory.
Complex metal hydrides, Dissolving metal reductions (including Birch, Benkeser), Diimide reduction, Organoboranes as reducing agents. McMurry reaction. Pummer, Willgerdot, Corey-Bakshi-Shibata and Tishchenko reactions.

**III Metallo enzymes 10 Hrs**

Structure and reactivity, Apoenzymes, Haloenzyme & Coenzyme. The principle involved and role of various metals in (i) Zn-enzymes: Carboxypeptidase, Carbonicanhydrase and alcoholdehydrogenase. (ii) Fe-enzyme: Catalase Peroxidase & Cytochrome P-450, (iii) Cu-enzyme: Superoxide dismutase (iv) Mo-enzyme: Oxatransferase enzymes, Nitrate reductase and Xanthine oxidase, Structure of vitamin B12, Co-enzyme Vit. B12, Coenzyme: B12r, B12s, biochemical functions of cobalamins, Co-C bond cleavage, Mutase activity of Co- enzyme B-12, Alkylation reactions of Methyl Cobalamin. Synthetic model of enzyme action, stability and ageing of enzyme.

**IV Electron Transfer in Biology 10 Hrs**

Electron transfer in Biology: Structure and functions of metalloproteins in electron transfer proteins, Cytochromes, Ferridoxines: 2Fe-2S, Rieske centers, High potential iron proteins; 4Fe-4S, 3Fe-4S, 8Fe-8S, Non-heme iron proteins; Rubredoxins, Synthetic models. Mitochondrial flow of electrons from NADH to oxygen, cytochrome C, Cytochrome C oxidase. Biological Nitrogen fixation (in vitro and in vivo)

**V Chemistry of Main Group Elements** **10 Hrs**

Chemistry of main group elements - Structure and bonding in boranes, carboranes, metallocarboranes, Wades rules, borazines, phosphazenes, S,N-compounds. Silicates-Classification, structures, isomorphous replacement, pyroxenes, layered and vitreous silicates, zeolites and molecular sieves.

**VI Isopoly and Heteropoly acids** **05 Hrs**

Isopoly and heteropoly acids of W, Mo and V, preparations, properties, structure and applications. Stereoisomerism - Chirality, optical activity.

**VII Nitrogenase** **05 Hrs**

Biological nitrogen fixation, molybdenum nitrogenase, spectroscopic and other evidence, other nitrogenases model systems.

**Reference Books**


1. Advanced Inorganic Chemistry, F.A. Cotton and Wilkinson, John Wiley.
2. Inorganic Chemistry, J.E. Huhey, Harpes & Row;
3. Chemisiry ol the Elements, N.N. Greenwood and A. Earnshow, Pergamon.
4. Comprehensive Coordination Chemistry eds., Q. Wilkinson, R.D. Gillars and J.A. McCleverty, Pergamon.
5. Biochemistry: The Chemical Reactions of Living Cells, D. E. MeUler, Academic Press.
6. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M. Berg, University Science Books.
7. Bioinorganic Chemistry, I. Bertini, H.B. Gray, S.J. Lippard and J.S. Valentine, University Science Books.
8. Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Hermann Dugas and C. Penny, Springer-Verlag.

**OR,**

# M.Sc. Semester-IV
# Elective (GE/DC) [EC-4]
# Organic Chemistry
### (Chemistry of Natural Products)
# Course Code : 1Y2CHE402

**Full Marks: 70+30**
**Total Lecture: 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Conformational Analysis** **10 Hrs**

Conformational analysis of simple cyclic (chair and boat cyclohexanes) and acyclic (n-butane) systems, conformation of simple 1,2 disubstituted derivatives - ethylene chlorohydrin and ethylene glycol, Conformational analysis and stereochemical features of disubstituted cyclohexanes (1,2- 1,3- 1,4- dialkylcyclohexanes), conformation and stereochemistry of cis- and trans-decalins, effects of conformation on reactivity in acyclic and cyclohexanes.

**II Terpenoids and Carotenoids** **10 Hrs**

Classification, nomenclature, occurrence, isolation, general methods of structure determination, isoprene rule.Structure determination, stereochemistry, biosynthesis and synthesis of the following representative molecules: Citral, α-Terpeneol, Zingiberene and β-carotene.

**III Structure Determination and Synthesis of Vit. A, $B_2$, $B_6$, Vit. C and Vit. D.** **10 Hrs**

**IV Six-Membered Heterocycles with Two or More Hetero-atoms** **10 Hrs**

Synthesis and reactions of Pyridazine, Pyrimidine and Pyrazine : Reactions with electrophilic reagents, oxidising agents, nucleophilic reagents, bases, C-metallated diazines, reducing reagents, electrocyclic and photochemical reactions, preparation of N-oxides.

**V Six-Membered Heterocycles with one Heteroatom** **10 Hrs**

**S**ynthesis and reactions of pyrytium salts and pyrones and their comparison with pyridiniurn & thiopyrylium salts. Synthesis and reactions of benzopyrylium salts.

**VI Alkaloids** **10 Hrs**

Definition, nomenclature and physiological action, occurrence, isolation, general methods of structure elucidation, degradation, classification based on nitrogen heterocyclic ring, role of alkaloids in plants. Structure, stereochemistry, synthesis and biosynthesis of the following : Atropine, Quinine, Morphine and Narcotine.

**VII Steroids** **10 Hrs**

Occurrence, nomenclature, basic skeleton, Diel's hydrocarbon and stereochemistry. Isolation, structure determination and synthesis of Cholesterol, Androsterone, Estrone, Progestrone, Biosynthesis of steroids.

**Reference Books**


1. The Chemistry of Heterocycles, T. Eicher and S. Hauptmann, Thieme.
2. Heterocyclic Chemistry, J. A. Joule, K. Mills and G.F. Smith, Chapman and Hall.
3. Comprehensive Heterocyclic Chemistry, A. R. Kalriliky and C. W. Rees, eds. Pergamon Press.
4. Natural Produds: Chemistry and Biological Significance, J. Mann, R. S. Davidson, J. B. Hobbs, D.V, Banthirope and J. B. Harbome, Longman,Essex.
5. Organic Chemistry, Vol 2, I. L. Finar, ELB S.
6. Mechanism and Theory in Organic Chemistry, T. H. Lowry and K. C. Richardson, Harper and Row.

## OR,
## M.Sc. Semester-IV
## Elective (GE/DC) [EC-4]
### Physical Chemistry
### (Electrochemistry)
## Course Code : 1Y2CHE402

**Full Marks: 70+30**
**Total Lecture : 70 Hours**

**Eight questions are to be set out of which five are to be answered.**

**I Electrochemistry** **15 Hrs**

Electrochemistry of solution, Debye-Huckel theory of strong electrolytes, Debye-Huckel-Onsager treatment and its extension, ion solvent interactions. Thermodynamics of electrified interface equations. Derivation of electro-capillarity, Lippmann equation (surface excess), methods of determination. Structure of electrified interface. Guoy-Chapman, Stern, Graham-Devnathan-Mottwatts, Tobin, Bockris, Devnathan models. Overpotentials, exchange current density, derivation of Butler-Volmer equation, Tafel plot. Quantum aspects of charge transfer at electrodes-solution interfaces, quantization of charge transtunneling.

**II Electrode Deposition** **10 Hrs**

Electrocatalysis - Electrocatalytic rate, Electrocatalysis in redox system. Total deposition current density, Time variation of the overpotential and rate determining step in electrode deposition. Total overpotential for electrode deposition in steady state. Hydrogen overvoltage, rate determining step of the hydrogen evolution reaction, Determination of reaction order with respect to $H^+$ ion in solution.

**III Corrosion Process** **15 Hrs**

Introduction, dry and wet corrosion, theories and mechanisms of wet (electrochemical) corrosion, thermodynamic aspects of corrosion, kinetic aspects- determination of rates of corrosion by linear polarization, Tafel extrapolation and impedance techniques. Factors influencing the rate of corrosion-metal and environmental. Methods of corrosion prevention: Cathodic protection, anodic protection, use of corrosion inhibitors, use of organic coatings.
Passivity: Definition, corrent potential diagram, characteristics of passivity, theory and mechanism of passivation, flade potential, trans passivity. Use of ellipsometric technique in the study of passivating films.

**IV Electrode Kinetics** **15 Hrs**

Faradic and non-Faradic current, Rate law, Current density, Factors affecting electrode reaction, Types of overvoltage, Polarisation, Polarisation curves, Electric potential, derivation of Nernst equation (i) On thermodynamic consideration and (ii) By kinetic approach, Nernst diffusion layer treatment, exchange current density, Stoichiometric number, Concept of rate determining step, Energy barriers for multistep reactions, Studies on electrode kinetics-polarographic analysis, Rotating disc convection method.

**V Catalysis and Oscillation** **15 Hrs**

Kinetics of catalytic reactions, Theory of acid-base catalysis, Vant Hoff and Arhensious complexes, Protogenic and protophillic mechanism, Effect of salt on acid-base catalysis, autocatalysis, Non-competitive and competitive inhibitors, Bronsted catalysis law, rate of reaction and acidity functions, Linear free energy relationship, Hammet equation, Meaning of substituent constant and reation constant in organic reactions, reactions in biological systems, Oscillating reaction, Lotka-Voltera model, B-Z reaction. The brus organator, bistability, Chemical chaos.

**Reference Books**


1. Physical Chemistry, Waller J. Moore
2. Physical Chemistry, P.W. Atkins
3. Thermodynamics for Chemists by S. Glasstone, East-West Press, New Delhi
4. Thermodynamics by Rajaraman and Kuriacose, East-West Press
5. Statistical Thermodynamics, M. C. Gupta (Wiley Eastern Ltd.)
6. Elementary Statistical Thermodynamics, N. D. Smith, Plenum Press, NY
7. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley
8. Modern Electrochemistry Vol-1 and 2, J. O. M. Bockris and A. K. N. Raddy, Plenum NewYork
9. An Introduction to Electrochemistry, Samuel Glastone East-West edition New Delhi
10. Text Book of Physical Chemistry, Samuel Glastone, 2nd edition, Mac Millan India Ltd.
11. Electrochemistry: Principles and Applications, Edmund, C. Potter, Cleaver, Hume press London
12. Principles and Applications of Electrochemistry, D. R. Crow, 3rd edition, Chapmanhall London

# M.Sc. Semester-IV
# EC(P)-5
## Inorganic Chemistry Practical
## Course Code : 1Y2CHE403P

**Full Marks: 100**
**Pass Marks: 50**
**Time : 12 Hrs**

Two questions are to be set.

**I Quantitative Analysis**

(i) Analysis of alloys (brass, type metal, solder, gun metal) cement, steel using conventional chemical analysis/and physical techniques (if possible). (Preferably one alloy and cement analysis may be carried out).

(ii) Analysis of two cation-system using complexones.

(iii) Colorimetric estimation of cation/anions.

**IISeparation Techniques**

(i) Ion exchange: Separation of inorganic cations/anions (2 or 3 components).

(ii) Chromatographic Separation.

(a) Cd-Zn (b) Zn-Mg

**III Preparation of simple inorganic complexes, their purification, Molecular Weight determination and elucidation of the structures by available physical methods.**

(a) Preparation of Cobalt (III) complexes

(i) $[Co(NH_3)_5Cl]Cl_2$

(ii) $[Co(NH_3)_5NO_2]Cl_2$

(iii) $[Co(NH_3)_5ONC]Cl_2$

(b) Preparation and characterisation of Cr(III) complexes

(i) $[Cr(H_2O)_6]NO_2.H_2O$

(ii) $[Cr(H_2O)_4Cl_2]Cl.H_2O$

(iii) $Cr(acac)_3$

(c) (i)Purification of inorganic complexes using techniques such as crystallisation, volatilisation etc.

(ii) Tests for purity-M.P., TLC, Metal analysis etc.

(d) Preparation and study of cis and trans isomers of bis (glycinato) copper(II)

(i) Cis-glycinato Cu(II) monohydrate

(ii) trans-glycinato Cu(II) monohydrate (IR sepectroscopy)

(e) Preparation of mercury tetrathiocyanato cobaltate : $Hg[Co(CNS)_4]$

**IV Determination of**

(a) Manganese/Chromium/Vanadium in steel sample by spectrophotometric method

(b) Ni/Mo/W/V/U by extractive spectrophotometric method.

**V Flame Photometric Determinations**

(a) Sodium and Potassium when present together

(b) Li/Ca/Ba/Sr Naphelometric determinations

(c) Sulphate (d) Phosphate (e) Silver

**Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.**

# M.Sc. Semester-IV
# EC(P)-5
## Organic Chemistry Practical
## Course Code : 1Y2CHE403P

**Full Marks: 100**
**Pass Marks: 50**
**Time: 12 Hrs**

Two questions are to be set.

**I Organic Systhesis and Extraction of Organic Compounds from Natural Sources:**

The students are expected to carry out 6 to 8 organic preparations/isolation (usually involving not more than two steps). Student should be asked to purify the crude sample, check the purity on a TLC single spot and/or get the pmr scanned and interpret.

Some of the illustrative experiments are listed below:

**Extraction:**

1. Extraction of Caffeine from Tea Leaves.
2. Isolation of Casein from Milk.
3. Isolation of Lactose from Milk.
4. Isolation of Nicotine dipicrate from Tobacco.
5. Isolation of Cinchonine from Cinchona bark
6. Isolation of β-Carotene from Carrots
7. Isolation of Oleic acid from Olive oil
8. Isolation of Eugenol from Cloves

**Preparation:**

1. Synthesis of 3-Nitrobenzoic acid from Benzoic acid.
2. Preparation of Indigo from Anthranilic acid.
3. Cannizzaro reaction of 4-Chlorobenzaldehyde.
4. Synthesis of Benzanilide from Benzene.
   Make a comparative study of the IR and PMR spectra of starting materials as well as producs, if possible.

**II Quantative Analysis:**

Some illustrative exercises are given below:

1. Estimation of phenol / aniline using bromate bromide solution/or acetylation method
2. Estimation of carbonyl group by using 2,4-dinitrophenyl hydrazine
3. To estimate nitrogen in the given sample by Kjeldahl method
4. To estimate sulphur in the given sample by the $Na_2CO_3$-$KNO_3$ fusion method.
5. To estimate sulphur in the given sample by Messenger's method.
6. To estimate a halogen in the given sample by the alkaline reduction method
7. To determine the percentage or number of hydroxyl groups in the given sample by the acetylation method.

**Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.**

# M.Sc. Semester-IV
# EC(P)-5
## Physical Chemistry Practical
## Course Code : 1Y2CHE403P

**Full Marks: 100**
**Pass Marks: 50**
**Time: 12 Hrs**

Two questions are to be set.

**I Chemical Kinetics**

1. To study the kinetics of alkaline hydrolysis of an ester in aquo-organic solvent system with respect to effect of solvent composition and dielectric constant on rate constant.
2. To determine the rate constant of the reaction between $K_2S_2O_8$ and KI at two different temp. and hence to determine the energy of activation of the reaction.

**II. Thermochemistry**

1. Determination of basicity of a polybasic acid.
2. Determination of heat of displacement of Cu by Zn from $Cu^{2+}$ salt solution.
3. Determination of heat of hydration of $Na_2SO_4$ to $Na_2SO_4$, 10 $H_2O$.

**III. Distribution law**

1. Determination of Composition of Cupric-ammine sulphate formed between $CuSO_4$ and $NH_3$
2. Determination of equilibrium constant for the reaction $KI+I_2=KI_3$

**IV. Thermodynamics and Surface Chemistry**

1. To study the adsorption of acetic acid on charcoal
2. To determine the partial molar volume of solutions of simple salts and to study its variation with concentration

**V.Viscosity and Surface Tension**

1. To determine the radius of a molecule from viscosity measurement.
2. To determine the parachor of - $CH_2$, C and H

**Practical-1: 40 Marks, Practical-2: 40 Marks, Note Book: 10 Marks, Viva: 10 Marks.**

# M.Sc. Semester-IV
# Course Code : 1Y2CHE404PR
# PROJECT

**Full Marks: 100**
**Time: 06 Hrs**

The paper will consist of

(a) Field work/Lab work related to the project.
(b) Preparation of dissertation based on the work undertaken.
(c) Presentation of project work in the seminar on the assigned topic in the University Department of Chemistry, DSPM University, Ranchi & open viva there on.

**NB**:- **The students will select topic for the project work in consultation with a teacher of the Department.**

## Topics

Project work related to the following Industrial/Social relevant topics may be given to the students of M.Sc. SEM-IV in Paper-XVI

(a) Environmental study such as
(i) Analysis of water, soil, air etc.

(b) Industrial goods analysis such as
(i) Analysis of Cement
(ii) Analysis of minerals/coal available in Jharkhand State
(iii) Synthesis of useful commercial products based on raw materials available in Jharkhand state such as Lac, lime-stone etc.
(iv) Isolation of constituents of Medicinal plants available Jharkhand State.

Each student has to submit two copies of the dissertation work duly forwarded by the HOD. The forwarded copies will be submitted in the University Department of Chemistry, YBN University, for evaluation (Seven days before the seminar).