



Department of Chemistry
University of Pune
Pune 411007

Structure of Syllabus
M.Sc. Part I & Part II
[2013-2014]

**STRUCTURE OF SYLLABUS
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF PUNE**

M.Sc. PART I

SEMESTER I

S.No.	Course	No. of Credits	No. of Lectures+ Tutorials/Seminar
1.	CHC – 100 : Mathematics for Chemists	2	24 + 06
2.	CHI – 120 : Symmetry, Group Theory and Spectroscopy	5	60 + 15
3.	CHO – 130 : Stereochemistry and Mechanism	5	60 + 15
4.	CHP – 140 : Kinetics and Thermodynamics in Chemistry	4	48 + 12

SEMESTER II

Optional Course (Any Two)

1.	CHC – 204(A) : Modern Separation Methods	2	24 + 06
2.	CHC – 204(I) : Chemistry of Main Group and Inner Transition Elements	2	24 + 06
3.	CHC – 204(O) : Heterocyclic Chemistry	2	24 + 06
4.	CHC – 204(P) : Radioactivity : Types, detection and applications	2	24 + 06

Compulsory Courses

5.	CHI – 220 : Coordination & Bioinorganic Chemistry	5	60 + 15
6.	CHO – 230 : Synthetic Organic Chemistry and Spectroscopy	5	60 + 15
7.	CHP – 240 : Chemical Bonding and Molecular Spectroscopy	5	60 + 15

Total Theory Courses : 8, No. of Credits Sem.I : 16 Sem. II : 19 = 35

PRACTICALS

5.	CHI – 127 : Experiments and computer applications in Inorganic Chemistry.	5	9 weeks
6.	CHO – 137 : Techniques, preparations and computer applications in organic chemistry	5	9 weeks
7.	CHP – 147 : Experiments and computer applications in physical chemistry	5	9 weeks

Total No. of Practical Courses : 3

15

Total No. of Theory + Practicals (35+15)

50

EVALUATION SYSTEM

1. Each course will have:
 - a. 50% of marks as semester-end examination of minimum 30 minutes to maximum 40 minutes per credit and
 - b. 50% marks for internal (i.e. in-semester) assessment.
2. The student has to obtain forty percent marks in the combined examination of In-Semester assessment and Semester-End assessment with a minimum passing of thirty percent in both these separately.
3. To pass, a student shall have to get minimum aggregate 40% marks (E and above on grade point scale) in each course.
4. Internal Assessment answer books may be shown to the students concerned but not the end-semester answer scripts.
5. While marks will be given for all examinations, they will be converted into grades. The semester end and final grade sheets and transcripts will have only grades and grade points average.
6. In subjects or departments where Project work is part of the credits, the Project will consist of not more than ten percent of the total credits for the degree course.
7. Each credit will have an internal (continuous) assessment of 50% of marks and a teacher must select a variety of procedures for examination such as:
 - i. Written Test and / or Mid Term Test (not more than one for each course);
 - ii. Term Paper;
 - iii. Journal/Lecture/Library notes;
 - iv. Seminar presentation;
 - v. Short Quizzes;
 - vi. Assignments;
 - vii. Extension Work;
 - viii. Research Project by individual students or group of students; or
 - ix. An Open Book Test (with the concerned teacher deciding what books are to be allowed for this purpose.)
8. The system of evaluation will be as follows: Each assignment/test will be evaluated in terms of grades. The grades for separate assignments and the final (semester-

end) examination will be added together and then converted into a grade and later a grade point average. Results will be declared for each semester and the final examination will give total grades and grade point average.

Marks	Grade	Grade Point
100 to 75	O: Outstanding	06
74 to 65	A: Very Good	05
64 to 55	B: Good	04
54 to 50	C: Average	03
49 to 45	D: Satisfactory	02
44 to 40	E: Pass	01
39 to 0	F: Fail	00

9. Final Grade Points :

Grade Points	Final Grade
05.00-6.0	O
04.50-4.99	A
03.50-4.49	B
02.50-3.49	C
01.50-2.49	D
00.50-1.49	E
00-00-0.49	F

10. Grade Point Average = $\frac{\text{Total of Grade Points Earned X Credit hrs for each course}}{\text{Total Credits Hours}}$

GPA (Grade Point Average) is calculated by taking the ratio of sum of credits obtained to sum of total credits (that is, 25 per semester). CGPA (cumulative Grade point average) will also be calculated in a similar manner considering all the courses enrolled from Semester I divided by 100 (which represents total number of credits).

11. 'B' Grade is equivalent to at least 55% of the marks as per circular No.UGC-1298/[4619]UNI-4 dated December 11, 1999.

12. The formula for GPA will be based on Weighted Average. The final GPA will not be printed unless a student passes courses equivalent to minimum 100 credits, 80 credits or 64 credits as the case may be.
13. A seven point grade system [guided by the Government of Maharashtra Resolution No. NGV-1298/[4619]/UNI.4 dt. December 11, 1999 and the University regulations] will be followed uniformly for Science. The corresponding grade table is detailed in II.14 above.
14. If the GPA is higher than the indicated upper limit in the three decimal digit, then the student be awarded higher final grade (e.g. a student getting GPA of 4.492 may be awarded 'A').
15. There will be only final compilation and moderation at (GPA (Final) level done at the Department. While declaring the result, the existing relevant ordinances are applicable. There is also a provision for verification and revaluation in case of verification, the existing rules will be applicable. The revaluation result will be adopted if there is a change of at least 10% marks and in the grade of the course.
16. The in-semester and end-semester examinations will be of 50% marks each . This will ensure that the students work regularly through the semester.
17. The description for each of the grades will be as follows:

Grade

Proposed Norms

O: Outstanding: Excellent analysis of the topic, (75% and above)

Accurate knowledge of the primary material, wide range of reading, logical development of ideas, originality in approaching the subject, Neat and systematic organization of content, elegant and lucid styl;

A: Very Good: Excellent analysis of the topic (65 to 74%)

Accurate knowledge of the primary material, acquaintance with seminal publications, logical development of ideas, Neat and systematic organization of content, effective and clear expression;

B: Good: Good analysis and treatment of the topic (55 to 64%)

Basic knowledge of the primary material, logical development of ideas, Neat and systematic organization of content, effective and clear expression;

C: Average: Some important points covered (50 to 54%)

Basic knowledge of the primary material, logical development of ideas, Neat and systematic organization of content, good language or expression;

D: Satisfactory: Some points discussed (45 to 49%)

Basic knowledge of the primary material, some organization, acceptable language or expression;

E: Pass: Any two of the above (40 to 44%)

F: Fail: None of the above (0 to 39%)

18. There will be an evaluation of each course by students at the end of every semester.
(*sample format enclosed for course evaluation by students*)

**Structure of Syllabus
Department of Chemistry
M.Sc. - Part I**

Semester I

CHC 100: Mathematics for Chemists

(2 Credits 24L+6 T/S)

1. Functions, differential and integral calculus, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, applications in chemistry, exact and inexact differential, Taylor and McLaurin series, curve sketching, partial differentiation, rules of integration, definite and indefinite integrals. (16L)
2. Differential equations
Separation of variables, homogeneous, exact, linear equations, equations of second order, series solution method. (04L)
3. Probability
Permutations, combinations and theory of probability (02L)
4. Vectors, matrices and determinants
Vectors, dot, cross and triple products, introduction to matrix algebra, addition and multiplication of matrices, inverse, adjoint and transpose of matrices, unit and diagonal matrices, (02L)

Text Books

1. The Chemical Maths Book, E. Steiner, Oxford University Press (1996).
2. Maths for Chemists, Volumes 1 and 2, Martin C. R. Cockett and Graham Doggett, Royal Society of Chemistry, Cambridge (2003).

Reference Books

1. Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill (1972).

CHI-120: Symmetry, Group Theory and Spectroscopy

(5 Credits, 60L)

A. Symmetry, Group Theory

1. Definitions and theorems of group theory, subgroups, classes. (3L)
2. Molecular symmetry and symmetry groups - symmetry elements and operations. Symmetry planes reflections, inversion centre, proper / improper axes and rotations, products of symmetry operations, symmetry point groups, classes of symmetry operations, classification of molecular point groups. (10L)

3. Representations of groups.

Great orthogonality theorem, character tables, properties of characters of representations. (5L)

4. Group theory and quantum mechanics. Wave function as bases for irreducible presentation. (2L)

5. Symmetry Adapted Linear Combinations - (SALC) - projection operators and their use to construct SALC. (4L)

6. Molecular Orbital Theory.

Transformation properties of atomic orbital's, MO's for Sigma bonding in AB_n molecules, tetrahedral AB_4 case, Hybrid orbital's, MO's for pi bonding in AB_n molecules. (6L)

7. Application of group theory to infrared spectroscopy (Ref.-2, Chapter-8)

Introduction, selection rules, polyatomic molecules, possible vibration in a linear molecule, bending modes, symmetry of vibrations and their IR activity, Group vibration concept and its limitations, IR spectra related to symmetry of some compounds, IR spectra of complex compounds. (6L)

B. Spectroscopy

1. Crystallographic - Unit cell, space lattice, Bravais lattices, Miller indices in cubic and hexagonal structure, crystallographic cubic volume density, planar density, linear density and percent transformation of polymorphism in crystal. (4L)

2. NMR: Fundamentals–Coupling, decoupling, first order analysis, second order coupling, relaxation processes. Structure determination of Inorganic systems having ^{11}B , ^{19}F , ^{31}P nuclei, factors influencing chemical shift and coupling constant, Dynamic Processes and NMR. (10L)

3. Mössbauer Spectroscopy: Basic principles, instrumentation, spectral parameter and displays, application

(a) Mössbauer parameters– Isomer shifts, quadrupole splitting, Magnetic hyperfine interaction, Doppler effect/shift.

(b) Application of Mössbauer Spectroscopy:

(i) Nature of chemical bonds in Prussian blue and Prussiates,

(ii) Covalently bonded compounds,

(iii) Oxidation states of metal ion in compounds,

(iv) Structural determination,

(v) Magnetically ordered compounds (i.e Ferromagnetic & antiferromagnetic compounds). (10L)

Books

1. Chemical applications and group theory F.A.Cotton, 3rd edition, John Wiley & Sons Asia Pvt. Ltd. (1999).
2. Group theory and its chemical applications: P.K Bhattacharya, 2nd edn, Himalaya pub. India, (1989).
3. Molecular symmetry and group theory -A. Vincent.
4. Symmetry in Chemistry: H.H.Jaffe' and M.Orchin, Dover Publications Inc, New York, (2002).
5. Symmetry in Inorganic Chemistry: J.P Fackler.
6. Principals of Materials Science and Engineering: William F. Smith (1980) (Chapter 3)
7. Physical Methods in Chemistry, R. S. Drago, Saunders, Harcourt Brac Javanovich College Publishers, (1992).
8. NMR spectroscopy in Inorganic Chemistry, J. A. Iggo, Oxford University press. (2001).
9. Mössbauer Spectroscopy and Transition Metal Chemistry, P. Gütllich,R. Link, A. Trautwien, Springer-Verlag (1978).
10. Mössbauer Spectroscopy, N.N. Greenwood, T.C. Gibb, Chapman and Hall Ltd. (1971).

CHO 130 Stereochemistry and Mechanism

(5 Credits+ 60L+15 T)

Organic Reaction Mechanism

- a. Acidity and basicity, aromaticity, Inductive, Mesomeric, steric effect, hyperconjugation, tautomerism and their influence on the properties of organic compound (8L)
- b. Nucleophilic Substitution Reactions at saturated carbon (10L)
- c. Addition and Elimination reactions (8L)
- d. Aromatic electrophilic and nucleophilic substitution Reactions (10L)
- e. Stereochemistry of Organic Compounds (15L)
- f. Non kinetic methods and Kinetic methods (9L)

Books

1. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and Winston)
2. Advanced organic chemistry by J. March, 6th Ed.
3. Advanced organic chemistry part-A. F. A. Carey and R. J. Sundberg, 5th Ed. Springer (2007)
4. Physical Organic chemistry – J. Hine
5. A guidebook to mechanism in organic chemistry – Peter Sykes 6th Ed. Orient Longman
6. The Hammett equation – C. D. Johnson, Cambridge University Press (1973)
7. Organic Chemistry – J. Clayden, N. Greeves, S. Warren and P. Wothers. Oxford University Press (2001)

CHP 140: Kinetics and Thermodynamics in Chemistry (4 credits, 48 L+12T)

Chemical Kinetics: (2 credits, 24L+6T)

Recapitulation:-

Rate of Reaction, Empirical Rate law, rate constants, order, molecularity, half-life and life time of reaction. Zeroth first and second and nth order reactions, method of integration. Differential and graphical methods to determine order of the reactions, The temperature dependence of reaction rates and Arrhenius rate equation (2L)

Solving rate laws for the Complex reactions:

Rate laws for complex reactions, parallel reaction with example of nuclear reactions and fluorescence decay, opposing reactions and evaluation rate constants by temperature jump method , consecutive reactions. (6 L)

Approximate methods to solve complex reactions:

Steady state and pre-equilibrium approximations, Lindemann mechanism for the unimolecular reaction. Enzyme catalysis_– Michaelis Menton Mechanism, with and without inhibitors, Lineweaver and Eadie plots, Chain reactions:_free radical polymerization, Explosions, reaction between H₂ and Br₂, depletion of O₃ layer, Autocatalysis and oscillating reactions (8 L)

Method of studying fast reactions:

Flash photolysis, stop flow technique, pump and probe methods (2 L)

Molecular reaction dynamics:-

Collision theory for bi-molecular reaction (derivation expected) the steric factor, limitation of collision theory.

Activated complex or Transition state theory for bimolecular reaction, Eyring equation (derivation expected), Potential Energy surface and reaction co-ordinates, Application of transition state theory for the reaction in solutions, diffusion controlled reaction, kinetic salt effect. Dynamics of molecular collisions, (6 L)

Text Books:

(1) Atkins' Physical Chemistry, Peter Atkins and Julio e Paula ninth edition Oxford University Press 2011.

(2) Physical Chemistry, D.A. McQuarrie, Viva Book private limited, 1998.

(3) Chemical Kinetics, K. J Laidler, Third edition, Pearson Education Inc., 1987.

Thermodynamics**(2 Credits, 24 L+6 T)****1. Recapitulation:**

Laws of thermodynamics , Maxwell's equations and their applications, equilibrium and spontaneity, partial molar quantities, chemical potential, ideal & non-ideal solutions, solute and solvent activity, chemical equilibrium, free energy change and equilibrium constant, ΔH , ΔS , ΔG & K and effect of temperature and pressure, partial molar quantities, chemical potential (10L)

2. Thermodynamics of real gases

Concept of activity, choice of standard states, Methods of determining activity coefficient and activity coefficient, variation of activity and activity coefficient of a gas with pressure and temperature, concept of fugacity, fugacity of a gas in mixture of real gases (6L)

3. Statistical thermodynamics

Molecular energy levels, Boltzmann distribution law, partition functions and ensembles, calculation of translational, rotational and vibrational partition functions, statistical thermodynamics and second law, calculation of different thermodynamic functions such as energy, heat capacity, entropy, free energy, equilibrium constants
(8L)

Reference Books:

1. Physical Chemistry, *P. W. Atkins*, Sixth Edition, Oxford University Press, Oxford (1998).
2. Physical Chemistry, *T. Engel and P. J. Reid*, Benjamin-Cummings (2005).
3. Physical Chemistry, *G. M. Barrow*, Fifth Edition, Tata McGraw Hill, New Delhi.

M. Sc. I Practicals

CHI-127: Experiments and computer applications in Inorganic Chemistry. (5 Credits, 9 weeks)

1. Ore Analysis: At least two of the following:
 - a. Determination of silica and manganese in pyrolusite .
 - b. Determination of copper and iron from chalcopyrite.
 - c. Determination of silica and iron from hematite
2. Alloy analysis (At least two of the following)
 - a. Determination of tin & lead from solder.
 - b. Determination of iron & Chromium from mild steel.
 - c. Determination of copper and nickel from cupronickel.
3. Inorganic Synthesis and purity determination (any five)
 - a. Cis-trans potassium di-aquo di-oxalato chromate (III)
 - b. Chloro penta-ammino cobalt (III) chloride
 - c. Nitro penta-ammino cobalt (III) chloride
 - d. Nitrito penta-ammino cobalt (III) chloride
 - e. Bis,2-4 pentanedionato cobalt (II) and cobalt (III)
 - f. Potassium tri-oxalato aluminate

4. Ion-exchange chromatography

Separation of mixture of Zn(II) and Mg(II) using Ammberlite IRA 400 anion exchanger and quantitative estimation of separated ions Zn(II) and Mg(II)

4. (a) Chelation in Nickel complexes: Preparation of Ni (II) ethylenediamine complexes and studying their absorption spectra.

(b) Solution state preparation of $[\text{Ni}(\text{en})_3]\text{S}_2\text{O}_3$, $[\text{Ni}(\text{H}_2\text{O})_6]\text{Cl}_2$, $[\text{Ni}(\text{NH}_3)_6]\text{Cl}_2$. Record the absorption spectra in solution of all three complexes and analyze it. Arrange the ligands according to their increasing strength depending on your observation

5. Instrumental methods of analysis.

a. Colorimetry.

1. Simultaneous determination of Cr & Mn.
2. Determination of K_{eq} of M-L Systems such as ,

Fe (III) - salicylic acid, Fe (III)-Sulphosalicylic acid
Fe (III) - β -resorcilic acid by Job's & Mole- ratio method.

- b. Determination of iron by solvent extraction technique in a mixture of Fe^{3+} + Al^{3+} & Fe^{3+} + Ni^{2+} using 8- hydroxyquinoline reagent.
- c. Study of aquation of $[\text{Fe}(\text{o-phen})_3]$ in acid solution by spectrophotometry.
- d. Conductometry (Ref.- 5)

i.Verification of Debye Hückle theory of ionic conductance for strong electrolytes KCl , BaCl_2 . K_2SO_4 , $\text{K}_3[\text{Fe}(\text{CN})_6]$

ii.Structural determination of metal complexes by conductometric measurement

iii. To study complex formation between Fe(III) with sulfosalicylic acid by conductometry

- e New Experiments : (any one)
- i. Data analysis, error analysis, least squares method. Plot of Born Maeyer to determine for 1:1 type molecule to determine internuclear separation. Characterization of metal ligand bonding using IR spectroscopy.
 - ii. Computer Applications: (1) Electronic structure, vibrational characteristics and charge distributions in first row transition metal complexes. (2) Visualizing frontier MO's.
 - iii. Analysis of Electronic spectra of transition metal complexes at least for one system ($d^n O_h$ or T_d) and calculation of Crystal Field parameters, inter electronic repulsion parameter and bonding parameter.

References:

1. Textbook of Quantitative Analysis, A. I. Vogel. 4th edn (1992).
2. Inorganic Electronic spectroscopy: A.B.P.Lever, 2nd edⁿ Elsevier Science Publishers, New York, (1984).
3. Inorganic Synthesis (Vol. Series)
4. Practical Manual made By Department of Chemistry, University of Pune
5. Experiments in Chemistry, D.V.Jahagirdhar, Himalaya Publishing House

CHO 137: Techniques, preparations and computer applications in organic chemistry

(5 credits, 9 weeks)

1. Techniques:

Crystallization, fractional crystallization, fractional distillation, vacuum distillation, sublimation, steam distillation, column chromatography, thin layer chromatography, gas chromatography, solvent drying (purity would be checked by m.p. and mixed m.p.) computational chemistry.

2. Preparation of derivatives.

Oxime, 2, 4 – DNP, acetyl, benzoyl, semicarbazide and aryloxyacetic acid,

3. Computer Application in Organic Chemistry

1. Drawing & Representation of Organic molecules using standard organic script & Bond Line Diagrams as per IUPAC recommendations.

2. Do & Don'ts of Stereochemical representations as per IUPAC recommendations.
3. Application of ISIS-Draw 2.4 (MDL INC freeware) & Chem Office 2011 for the generation of standard organic script as per IUPAC recommendations. Speciality applications in Chem Office 2011.

Standard References

1. Vogel Practical Organic Chemistry
2. Graphical Representation Standards for Chemical Structure Diagrams (IUPAC Recommendations 2008)
Prepared for Publication by
JONATHAN BRECHER, Cambridge Soft Corporation, 100 Cambridge Park Drive,
Cambridge, MA 02140, USA, Pure Appl., Chem., Vol.80, No.2, pp.277-410, 2008.,
rdoi:10.1351/pac200880020277
3. Graphical Representation of Stereochemical Configuration, (IUPAC Recommendations 2006)
Prepared for publication by
International Union of Pure and Applied Chemistry, Chemical Nomenclature and
Structure Representation Division
Jonathan Brecher, Pure Appl. Chem., Vol.78, No.10, pp.1897-1970,2006
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CHP 147: Experiments and computer applications in physical chemistry (5 Credits 9 weeks)

Conductometry:

1. Hydrolysis of NH_4Cl or H_3COONa or aniline hydrochloride
2. Solubility of a sparingly soluble salt.
3. Hydrolysis of ethyl acetate by NaOH .
4. Determination of ΔG , ΔH , and ΔS of Silver Benzoate by conductometry.

Potentiometry:

1. Stability constant of a complex ion.
2. Solubility of a sparingly soluble salt.
3. Determination of dissociation constant of acetic acid.
4. Estimation of halide in mixture.
5. pH metry.
6. Hydrolysis of aniline hydrochloride.
7. Determination of the acid and base dissociation constants of an amino acid and hence the isoelectric point of the acid.
8. To determine the amount of aspirin in the given tablet.

Colorimetry:

1. Analysis of a binary mixture.
2. Copper EDTA photometric titration.
3. Determination of stability constant of ferric salicylate complex by colorimetric measurements

Radioactivity:

1. Half-life of a radioactive nuclide.
2. Determination of E_{\max} of beta radiation and absorption coefficients in Al.
3. Counting errors.

Chemical kinetics:

1. Kinetic decomposition of diacetone alcohol by dilatometry.
2. Determination of an order of a reaction.
3. Bronsted primary salt effect.
4. Kinetics of the reduction of methylene blue by ascorbic acid.

Non-Instrumental:

1. Freundlich and Langmuir isotherms for adsorption of acetic acid on active charcoal.
2. Molecular weight by steam distillation.
3. Glycerol radius by viscosity.
4. Partial Molar volume (Pycnometry)
5. Determine the viscosities of mixtures of different compositions of liquids and find the composition of a given mixture.

Computer applications:

1. Least square fitting of experimental data.
Each candidate should perform a minimum of 20 experiments with at least two experiments from each technique.

Text Books

- (1) Findlay's Practical Physical Chemistry, B. P. Levitt and J.A. Kitchener 9th Edition, Longmans, London (1972).
- (2) Experiments in Physical Chemistry by J. M. Newcombe, R. J. Denaro, A. R. Rickett, R.M.W Wilson, Pergamon (1962).
- (3) Senior Practical Physical Chemistry, 5th Edition, B. D. Khosla, V. S. Garg and A. Khosla, R. Chand (1987).

**STRUCTURE OF SYLLABUS
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF PUNE**

M.SC. PART I

SEMESTER II

CHC - 204 (A) : Modern Separation Methods

(2 Credits, 24 L+6T)

1. Chromatography

12L

Partition chromatography: theory, uses and examples.
Adsorption chromatography: Types of adsorption chromatography.
Operation of columns, elution, supports
Thin layer chromatography
High Performance Thin Layer Chromatography: its advantages and uses
Gas chromatography: its advantages and uses.
Gel chromatography: theory, materials used, advantages and applications.
High performance liquid chromatography and its applications
Ion exchange chromatography: principles, properties of ion exchangers, choice of ion exchangers, porosity and mesh size, capacity, choice of pH, buffer and ionic conditions. Applications of ion exchange chromatography. Mixed Mode RP-LC separations (with ion chromatography): cation separations, mobile phase chemistry with a counter-ligand, post column reagent (PAR) chemistry to enhance sensitivity, mixed mode chemistry – ion exchange and hydrophobic interactions, micelles and surfactants
Affinity chromatography and its applications.

2. Hydrodynamic methods

4L

Sedimentation, simple theory of velocity-sedimentation.
Instrumentation for ultracentrifugation.
Analytical and preparative ultracentrifuge.
Boundary-sedimentation-velocity experiment.
Factors affecting sedimentation velocity.
Zonal centrifugation through reformed density gradient.
Determination of molecular weight by sedimentation.

3. Electrophoresis and Isoelectric focusing

4L

Theory of electrophoresis, types of electrophoresis: electrophoretic migration, capillary electrophoresis, electro-osmotic flow, BB behavior and separation optimization moving boundary and zone electrophoresis, paper electrophoresis, cellulose acetate strip and polyacrylamide gel electrophoresis, SDS-PAGE- vertical and horizontal electrophoresis and their applications, 2D Gel electrophoresis. Agarose gel electrophoresis and its applications. Isoelectric focusing its theory and applications. Micellar electrokinetic chromatography, Fingerprinting and large-scale preparative

electrophoresis. Applications in Nucleic acids, Clinical and capillary zone electrophoresis of carbohydrates.

4. Hyphenated Techniques

4L

Mass spectrometry principle, Instrumentation, Ionization methods –EL, CI, FAB, arc & spark, photoionization, thermal ionization, FI*&FD, laser induced, Photoelectric ionization, SIMS, Mass analyzers –Magnetic, Double focusing, Time of flight, Quadrupolar, Ion cyclotron resonance analyzer. Coupled techniques, GC FTIR, GCMS (Use of stable isotopes) HPLC-MS, LC-MS/MS, HPCCC (High Performance counter current chromatography)

Books:

1. Practical Aspects of Gas Chromatography
G.M.Message, John Wiley & Sons, New York (1984)
2. HPLC: Analytical Chemistry by Open Learning 2nd edition Sandie Lindsay Ed.
John Wiley & Sons, New York (1991)
3. Principles of Analytical Chemistry, Douglas Skoog, F.J. Holler and S.R.Crouch 6th edition, Thomson Brooks/Cole, 2007.
4. Physical Biochemistry: Applications to Biochemistry and Molecular Biology 2nd ed.
David Freifelder, W.H Freeman Publisher (1982)

CHC – 204(I) : Chemistry of Main Group and Inner Transition elements

(2 Credits, 24L+6T)

(a) Main Group elements:

1. Hydrogen & its compounds (2L)

Hydrides → classification, e⁻ deficient, e⁻ precise & e⁻ rich hydrides PH₃, SbH₃, AsH₃, Selenides, Tellurides.

2. Alkali & alkaline earth metals (2L)

Solutions in non-aqueous Media. Application of crown ethers in extraction of alkali & alkaline earth metals.

3. Organometallic compounds of Li, Mg, Be, Ca, Na (2L)

Synthesis, properties, uses & structures.

4. Boron group (3L)

Boron Hydrides, preparation, structure & bonding with reference to LUMO, HOMO, interconversion of lower & higher boranes, Metalloboranes, Carboranes.

5. Carbon group (3L)

Allotropes of Carbon, C₆₀ and compounds (fullerenes), Intercalation compounds of Graphite, Carbon nanotubes, synthesis, properties, structure-single walled, multiwalled, applications, classification of organometallic compounds. Organometallic compounds of B, Si, Sn,Pb, Ga, As, Sb, Bi. Structures, Synthesis, Reactions

6. Nitrogen group (3L)

Nitrogen activation, Boron nitride, Oxidation states of nitrogen & their nterconversion PN & SN compounds NO_x & their redox chemistry

7. Oxygen group (2L)

Metal selenides & tellurides, oxyacids & oxoanions of S & N, Ring, Cage and Cluster compounds of p-block elements. Silicates, including Zeolites

8. Halogen group (3L)

Interhalogens, Pseudohalogen, synthesis, properties & applications, structure, oxyacids & oxoanions of Hallogens Bonding.

9. Noble gases (1L)

Synthesis, properties, uses, structure & bonding with respect to VSEPR.

(b) Inner Transition elements with respect to oxides, halides and oxyhalides only (3L)

Ref. 3 Sc (page 689-692), V (page 701-710), Cr (page 718-728), Mn (page 739-748), Fe (page 763-774), Co(page 787-794), Ni (page 805-814), Cu (page 822-832), Zn (page 842-843)

Books:

1. Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson, C. A. Murillo, M. Bochmann, 6th edn. (2003).
2. Inorganic Chemistry: D. F. Shriver and P.W. Atkins, 4th edn. Oxford (2003).
3. Concise inorganic Chemistry, J.D.Lee 4th edition (Chapman and Hall)

CHC – 204(O) : Heterocyclic Chemistry (2 credits, 24 L+6T)

Heterocyclic chemistry – Structure, properties, reaction and synthesis of Pyrrole, Furan, Thiophene, pyridine, quinoline, isoquinoline, indole, benzofuran, imidazole, thiazole, pyrimidine and purines. (24L)

Books

1. Modern Heterocyclic chemistry – L. A. Paquette (Benjamin).
2. Heterocyclic chemistry – 3rd edition Raj K. Bansal, New Age International (P) Ltd. (1999).
3. Heterocyclic chemistry – J. A. Joule and K. Mills 4th edition Blackwell publishing (2007)

CHC - 204 (P) : Radioactivity: Types, detection and applications (2 Credits 24 L+6T)

Radioactivity: General Characteristics of radioactive decay, decay kinetics, theory of alpha, beta and gamma decay (6 L)

Radiation detection: Behavior of an ion pair in an electric field, classification of detectors, Gas filled detectors: ionization chamber, proportional counter, G.M.Counter; Scintillation counter (6 L)

Applications of Radioisotopes: General principles, applications in various fields-
Chemical investigations: reaction mechanism, structure determination, Physicochemical applications: surface area of powder, diffusion coefficient, Medical applications: thyroiditis, volume of blood, Analytical applications: neutron activation analysis, isotope dilution analysis, radiometric titrations, Industrial applications: gamma radiography (12 L)

References

1. Essentials of Nuclear Chemistry, H. J. Arnikar, Wiley Eastern Limited, 4th Edition.(1995)
2. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy and J. M. Miller, John Wiley (1981)
3. Sourcebook on Atomic Energy-S. Glasstone, Van Nostrand Company (1967)

CHI- 220: Coordination & Bioinorganic Chemistry (5Credits, 60L+15T)

(a) Coordination Chemistry

1. Concept & Scope of ligand Fields. (1L)
2. Energy levels of transition metal ions, Free ion terms, spin –orbit coupling. (7L)

3. Effect of ligand fields on energy levels of transition metal ions, weak cubic ligand field effect on Russell-Saunders terms, strong field effect, correlation diagrams, Tanabe-Sugano diagrams, Spin-pairing energies. (8L)
4. Electronic spectra of complexes, band intensities, band energies, band width & shapes, spectra of 1st, 2nd & 3rd row ion and rare earth ion complexes, spectrochemical & Nephelauxetic series, charge transfer & luminescence spectra, calculations of Dq, B, β parameters. (8L)
5. Magnetic properties of complexes, paramagnetism, 1st & 2nd ordered Zeeman effect, quenching of orbital angular momentum by Ligand fields, Magnetic properties of A,E,T ground terms in complexes, spin free–spin paired equilibria (6L)

(b) Bioinorganic Chemistry

6. Overviews of Bioinorganic Chemistry. (2L)
7. Principles of coordination Chemistry related to Bioinorganic–Proteins, nucleic acids and other metal binding biomolecules 6L
8. Choice, uptake and assembly of metal containing units in Biology (6L)
9. Control and utilization of metal ion concentration in cells. (6L)
10. Metal ion folding and cross –linking of biomolecules. (6L)
11. Binding of metal ions and complexes to biomolecular active Centers (4L)

Books:

1. Ligand field theory & its application: B.N.Figgis & M.A.Hitchman Wiley VCH publ. (2000), Chapters 5, 6, 8,9,11.
2. Principles of Bioinorganic Chemistry: S.J.Lippard & J.M Berg, University science books, Mill Valley, California (1994), Chapters- 1,2,3,5,6,7,8.
3. Inorganic Chemistry: D. F. Shriver & P. W. Atkins, Oxford (1999).
4. Inorganic Electronic spectroscopy: A.B.P.Lever, 2nd edⁿ Elsevier Science Publishers, New York, (1984).
5. Biological Chemistry of the Elements: R. J. P. Williams & F. R. DeSalvia, Oxford University Press-(1991).
6. Bioinorganic Chemistry: Inorganic elements in the Chemistry of life: An introduction & guide: W.Kaim, B.Schwederski, VCH, (1991).

CHO 230: Synthetic Organic chemistry and Spectroscopy (5 credits, 60L+ 15T)

1. Oxidation and Reduction (16L)
2. Reactive intermediates & molecular rearrangements (8L)
3. Ylids & organo-metallic chemistry (10L)
4. Spectroscopic methods for structure determination organic Compounds (16L)
5. Hammett equation (10L)

Books

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 3rd Ed. (Harcourt college publishers).
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, 6th Ed. John Wiley and Sons.
3. Spectroscopic methods in organic chemistry - D. H. Williams and I. Fleming Mc Graw Hill
4. Absorption spectroscopy of organic molecules – V. M. Parikh
5. Nuclear Magnetic Resonance – Basic Principles- Atta-Ur-Rehman, Springer-Verlag (1986).
6. One and Two dimensional NMR Spectroscopy – Atta-Ur-Rehman, Elsevier (1989).
7. Organic structure Analysis- Phillip Crews, Rodriguez, Jaspars, Oxford University Press (1998)
8. Organic structural Spectroscopy- Joseph B.Lambert, Shurvell, Lightner, Cooks, Prentice-Hall(1998).
9. Organic structures from spectra –Field L.D., Kalman J.R. and Sternhell S. 4th Ed. John Wiley and sons Ltd.

CHP-240: Chemical Bonding and Molecular Spectroscopy (5 Credits, 60 L+15T)

Chemical Bonding

1. Recapitulation, quantization, Postulates of Quantum mechanics, Schrödinger equation, particle in a box, particle in 3-D box, degeneracy, hydrogen-like atoms (no derivation), atomic orbitals. (12 L)
2. Variational method, many electron atoms, orbital angular momentum, electron spin, wave functions of many electron atoms, Pauli exclusion principle, spin-orbit interaction, fine structure, vector atom model, spectral terms. (5 L)

3. Molecular orbital theory, Born-Oppenheimer approximation, H₂ molecule, homo- and hetero-nuclear diatomic molecules, MO diagrams of simple triatomic molecules. (5 L)
4. Valence bond theory of simple molecules, quantitative treatment of hydrogen molecule and related systems, hybridization, comparison of VBT and MOT. (4 L)
5. Hückel theory of conjugated hydrocarbons, Electron densities, Bond orders and free valence indices, Illustrations (6 L)

Text Books

1. Quantum Chemistry, I. Levine, 5th Edition, Prentice Hall (1999).

Reference Books

1. Valence, C. A. Coulson, ELBS (1974).
2. Introduction to Quantum Mechanics- with Applications to Quantum Chemistry, L. Pauling and E. B. Wilson, Dover Publishers (1999).
3. Orbitals in Chemistry, V. Gil, Cambridge University Press (2000).

Molecular Spectroscopy

1. Recapitulation, regions of electromagnetic spectrum, width and intensity of spectral lines. (2 L)
2. Rotational spectra: classification of molecules based on the moment of inertia, Schrodinger equation of rigid rotor, diatomic molecules, effect of isotopic substitution, centrifugal distortion, linear triatomic molecules, symmetric top molecules, stark effect. (5 L)
3. Infrared spectra: quantum mechanical harmonic oscillator, diatomic molecule, Morse potential, overtone and hot bands, polyatomic molecules, skeletal and normal vibrations (6 L)
4. Vibrational rotational spectra, fine structure in diatomic molecules, break down of the Born-Oppenheimer approximation, effect due to nuclear spin, parallel and perpendicular vibrations. (4 L)
5. Raman Spectra: classical and quantum theory of Raman effect, stokes and antistokes lines, polarizability ellipsoid, rotational Raman spectra, selection rule, vibrational raman spectra, rule of mutual exclusion, elucidating structure from the combined infrared and Raman spectra, rule of mutual exclusion (6 L)
6. Electronic spectra: Born-Oppenheimer approximation, molecular progression, term symbols, Franck-Condon principle, dissociation energies, oscillator strength, rotational fine structure, fortrat parabola, predissociation, photoelectron spectroscopy (5 L)

Text Books

- 1) Fundamentals of Molecular Spectroscopy, C. M. Banwell and E. McCash, Tata McGraw Hill, 4th Edition (1994).
- 2) Molecular Spectroscopy, J. Machale, Prentice Hall, NJ, USA (1999).
- 3) Vibrating Molecules, P. Gans, Chapman and Hall, UK (1971).

**STRUCTURE OF SYLLABUS
DEPARTMENT OF CHEMISTRY
UNIVERSITY OF PUNE**

M.SC. PART II

Semester III:

Analytical Chemistry Sem. III

Course No.	Course name	Credits	Total credits per sem.
Compulsory courses			19
CHA- 350	Principles and Applications of Analytical science	5	
CHA- 351	Advanced Analytical Techniques	5	
CHA- 352	Analytical Chemistry of Pharmaceuticals and Polymeric materials	5	
CHA- 353	Clinical and Consumer Product Analysis	4	

M. Sc. Inorganic Chemistry: Theory

	Course No.	Compulsory courses	Total credit per sem	Total credits per sem.
Sem.- III	CHI-320	Physical methods of coordination compounds and Bio-inorganic chemistry	5	20
	CHI-321	Inorganic reaction mechanism and Photochemistry	5	
	CHI-322	Organometallic chemistry and Homogeneous catalysis	5	
	CHI-323	Frontier's in material science and technology and characterization by Analytical methods	5	

M. Sc. Organic Chemistry: Theory

	Course No.	Compulsory courses	Total credit per sem	Total credits per sem.
Sem.- III	CHO-330	Carbanion, NGP and retro synthetic analysis	4	19
	CHO-331	Spectroscopic Methods in Structure Determination	5	
	CHO-332	Stereochemistry	5	
	CHO-333	Pericyclic Reactions, photochemistry and Free Radical Chemistry and their applications in organic synthesis	5	

M. Sc. Physical Chemistry: Theory

Semester III			
Course No.	Course Name	Credits	Total credits per sem.
Compulsory Courses			19
CHP 340	Quantum Chemistry	5	
CHP 341	Nuclear, Radiation and Photochemistry	5	
CHP 342	Physicochemical Methods of Analysis and Computer Programming	5	
Optional Courses Any One From Following			
CHP 343	QSAR and Molecular Modeling	4	
CHP 344	Polymer Materials : Principles and Processing	4	
CHP 345	Molecular Reaction Dynamics and Non-Equilibrium Thermodynamics	4	

M. Sc. III Practicals

Course No.	Course Name	Credits	Total credits per sem.
Analytical Chemistry			
CHA- 358	Analytical Chemistry Practicals I	4	8
CHA- 359	Analytical Chemistry Practicals II	4	
Inorganic Chemistry			
CHI-328	Inorganic Chemistry Practicals- I	4	8
CHI-329	Inorganic Chemistry Practicals- II	4	
Organic Chemistry			
CHO- 337	Mixture Separation	4	8
CHO-338	Advanced Preparation	4	
Physical Chemistry			
CHP-346	Experiments in physical chemistry I	4	8
CHP-347	Experiments in physical chemistry II	4	

M.Sc. PART II
Semester IV:
Analytical Chemistry Sem. IV

Course No.	Course name	Credits	Total Credits per Sem.
CHA- 450	Industrial Products and Forensic Analysis	6	
CHA- 451	Pharmaceutical Analytical Chemistry	6	

M. Sc. Inorganic Chemistry: Theory

	Course No.	Compulsory courses	Total credit per sem	Total credits per sem.	
Sem.-IV	CHI-420	Inorganic polymer , clusters and Heterogeneous catalysis	5	14	
	CHI-421	Inorganic material chemistry	5		
	Elective Courses				
	CHI-423	Inorganic applications in industry and medicine	4		

M. Sc. Organic Chemistry: Theory

	Course No.	Compulsory courses	Total credit per sem	Total credits per sem.
Sem.-IV	CHO-430	Synthetic Organic Chemistry	6	16
	CHO-431	Advanced Chemistry of Natural products	6	
	CHO-434	Biogenesis of Organic Compounds (Intersectional option)	4	
	CHO-454	Organic Polymers and Agrochemicals	2.5	

M. Sc. Physical Chemistry: Theory

Course No.	Course Name	Credits	Total credits per sem.
Compulsory Courses			16
CHP 440	Resonance Spectroscopy and Magnetochemistry	4	
CHP 441	Solid State Chemistry and Electrochemistry	4	
CHP 442	Surface Chemistry and Catalysis	4	
Optional Courses Any One From Following			
CHP 443	Advanced Quantum Chemistry	4	
CHP 444	Special Topics in Nuclear and Radiation Chemistry	4	
CHP 445	Nanoscale Materials Science	4	
CHP 446	Advanced Electrochemistry	4	

Project

Compulsory Course Project		
CHA- 458	Project Work	7
CHI- 428	Project Work	7
CHP- 447	Project Work	7
CHO- 427	Project Work	7