Central University of Punjab, Bathinda

Course Scheme & Syllabus

M.Sc. Chemistry (Computational Chemistry)

Session: 2018-20

Semester-I

S. No.	Course Code	Course Title	Course Type	Hours			
				L	T	P	Cr
1	CCC.506	Fundamental Biology	CF	2	-	-	2
2	CCC.507	Mathematics for Chemists	CF	3	1	-	4
3	CCC.512	Computational Methods	CC	3	1	-	4
4	CCC.508	Scientific Programming	CF	3	1	-	4
5	CHM.511	Physical Chemistry-I	CC	3	-	-	3
6	CCC.515	Scientific Programming	CC	-	-	6	3
		(Practical)					
7	XXX	Interdisciplinary Elective	IDE	2	-	-	2
8	CHM.509	Inorganic Chemistry-I	DSE	3	-	-	3
9	CHM.510	Organic Chemistry-I	DSE	3	-	-	3
10	CCC.513	Statistics for Chemical and	DSE	3	-	-	3
		Biochemical Applications					
11	CCC.514	Physical Organic Chemistry	DSE	3	-	-	3
10	CCC.516	Chemistry without test tube	IDE	2	-	-	2
	Total			25 Credits			

Semester-II

S. No.	Course Code	Course Title		Course Type	Hours			
					L	T	P	Cr
1	CCC.526	Quantum Chemistry - I		CC	3	1	-	4
2	CCC.524	Statistical Mechanics - I		CC	3	1	-	4
3	CHM.523	Physical Chemistry-II		CC	3	-	-	3
4	CHM.525	Molecular Spectroscopy		CC	3	-	-	3
5	CCC.527	Physical Chemistry–II		CC	-	-	4	2
		(Practical)						
6	CCC.528	Computational Methods	Lab	CC	-	-	6	3
		(Practical)						
7	CCC.542	Seminar 1		SBE	-	-	-	1
8	XXX	Interdisciplinary Elective		IDE	2	-	-	2
9	CHM.521	Inorganic Chemistry-II		DSE	3	-	-	3
10	CHM.522	Organic Chemistry-II		DSE	3	-	-	3
11	CCC.529	Density Functional Theory		DSE	3	-	-	3
12	CCC.530	Introduction to Quantum		DSE	3	-	-	3
		Dynamics						
	Total			25 Credits				

Mode of Transaction

Lecture, Seminar, Group discussion, Team teaching, Self-learning.

Evaluation Criteria

As per UGC guidelines on adoption of CBCS.

Semester III

S. No.	Course Code	Course Title	Course Type	Hours			
				L	T	P	Cr
1	CCC.556	Electronic Structure Theory	CC	3	1	-	4
2	CCC.554	Fundamentals of Molecular Simulations	CC	4	-	-	4
3	CCC.555	Molecular Simulations Lab (Practical)	CC	-	-	6	3
4	CCC.553	Bioinorganic and Biophysical Chemistry	CC	3	-	-	3
5	CCC.599	Project	SBE	-	-	-	6
6	XXX	Value Added Course	EF	1			1
	Total						21

Semester IV

S. No.	Course Code	Course Title	Course Type	Hours			
				L	T	P	Cr
1	CCC.571	Biomolecular(Practical) Modeling Lab	CC	-	-	6	3
2	CCC.572	Electronic Structure Theory(Practical) Lab	CC	-	-	6	3
3	CCC.599	M. Sc. Project Work - II	SBE	-	-	-	6
4.	XXX	Value Added Course	EF	1			1
5	CCC.573	Biomolecular Modeling	CC	4	-	-	4
6	CCC.544	Seminar-II	SBE	-	-	-	1
7	CCC.577	Enrich Chemistry Course-I	CF	-	2	-	2
8	CCC.578	Enrich Chemistry Course-II	CF	-	2	-	2
				22 Credits			

Mode of Transaction
Lecture, Seminar, Group discussion, Team teaching, Self-learning.

Core Course, VAC: Value Added Course, EP: Elective Project, SEC: Skill Enhancement Course, IDE: Interdisciplinary Course, DSE: Discipline Specific Course, EF: Elective Foundation, CF: Compulsory Foundation, DEC: Discipline Enrichment Course; SBE: Skill Based Elective

*Students must take some MOOCs for a minimum total of 4 credits between 1st and 3rd semester.

SEMESTER- I

Course Title: Fundamental Biology
Paper Code: CCC.506
Total Lectures: 30

L	T	P	Cr
2	0	0	2

Course Objective and Learning Outcomes: To impart knowledge of molecular structure and interactions present in various bio-molecules that assist in functioning and organization of biological cell. After, completion of this course the students will acquire knowledge of molecular structure and interactions present in proteins, nucleic acids, carbohydrates and lipids, the organization and working principles of various components present in living cell, and the physical principles of structure, function, and folding of biomolecules.

Unit-I 7 hours

Introduction: Cell structure and functions, thermodynamics and kinetics of biological processes, ATP. water – physical properties and structure of water molecules, Interactions in aqueous solutions, Role of water in life, pH, Biological buffers, solution equilibria, Henderson-Hasselbalch equation, Hofmeister series, Chaotropic and kosmotropic ions/co-solvents.

Unit-II 7 hours

Amino Acids and Peptides: Classification and properties of amino acids, peptide and polypeptides, primary structures, structure of peptide bond, synthesis of peptides, N-terminal, C-terminal and sequence determination. Carbohydrates: Biologically important monosaccharides, disaccharides and polysaccharides, glycoproteins, role of sugars in biological recognition.

Unit III 8 hours

Proteins: Secondary structure of proteins with emphasize on supramoelcular characteristics of -helix, -sheets, supersecondary structure and triple helix structure of collagen, tertiary structure of protein-folding, quaternary structure of protein, protein misfolding and conformational diseases.

Catalysis and binding in enzymes, ligand-protein interactions, membranes, ribosomes and multienzyme complexes as supramolecular complexes.

Unit IV 8 hours

Nucleic Acids: Purine and pyrimidine bases, nucleotides, nucleosides, base pairing via H-bonding, structure of ribonucleic acids (RNA) and deoxyribonucleic acids (DNA), double helix model of DNA, different types of RNA and their functions, the chemical basis for heredity, overview of replication of DNA, transcription, translation and genetic code, genome sequencing and PCR techniques.

Lipids: Lipid classification, lipid bilayers, liproproteins-composition. high density (HDL) and low-density (LDL) lipoproteins and function, membrane

proteins - integral membrane proteins, lipid linked proteins, peripheral proteins, overview of membrane structure and assembly, liposomes, their biological functions.

Suggested Readings

1. Voet, D.J., Voet, J.G., Pratt, C.W., Principles of Biochemistry, 3rd edition, 2008, John Wiley,
2. Berg, J.M., and Tymoczko, J.L., Stryer, L., Biochemistry, 6th edition, 2007, W.H. Freeman,.
3. Garrett, R.H., Grisham, C.M., Biochemistry, Brooks/Cole, 4th edition, 2014, Cengage Learning,.
4. Conn, E.E., and Stump, F., Outlines of Biochemistry, 5th edition, 2006, John Wiley.

Course Title: Mathematics for Chemists
Paper Code: CCC.507
Total Lectures: 60

L	T	P	Cr
3	1	0	4

Course Objective and Learning Outcomes: The objective of this course is to cover the basic mathematical techniques that are commonly used by chemist. After, completion of this course will help the students to solve the complex problems in group theory, quantum chemistry, statistical thermodynamics, molecular spectroscopy, and chemical kinetics etc in the advance stage of computational chemistry program.

Unit I: Vectors, matrices and determinants 15 hours

Vectors: Vectors, dot, cross and triple products etc. the gradient, divergence & curl, vector calculus. Applications:
Two body peoblem, center of mass and relative coordinates, Potentials. Matrix algebra: addition and multiplication, inverse, adjoint and transpose of matrices, special matrices (symmetric, skew symmetric, hermitian, skew hermitian, unit, diagonal, unitary etc) and their properties, matrix equations: homogeneous, non homogeneous linear equations and conditions for the solution, linear dependence and indepedence, introduction to vector spaces, matrix eigenvalues and eigenvectors, diagonalization, determinants, introduction to tensors. Applications: Slater determinants, Huckel Molecular Orbital Theory, Polarizability and Magnetic Susceptibility.

Unit II: Differential calculus 15 hours

Functions, continuity and differentiability, rules for differentiation, applications of differential calculus including maxima and minima, exact and inexact differentials with their applications to thermodynamic properties. Applications: Maximally populated rotational energy levels, Bohr's radius and most probable velocity from Maxwell distribution.

Unit III: Integral calculus 14 hours

basic rules for integration, integration by parts, partial fraction and substitution, reduction formulae, applications of integral calculus, functions of several variables, partial differentiation, co-ordinate transformations
Applications: Cartesian to spherical polar, curve sketching.

Unit IV: Elementary differential equations: 16 hours
variables-separable and exact first-order differential equations, homogeneous, exact and linear equations, solutions of differential equations by the power series method, Fourier series, solutions of harmonic oscillator and legendre equation etc, spherical harmonics, second order differential equations and their solutions. Applications: chemical kinetics, secular equilibria, quantum chemistry etc,
Permutation and probability: permutations and combinations, probability and probability theorems, probability curves, average, root mean square and most probable errors, example from the kinetic theory of gases etc, curve fitting (including least squares fit etc) with a general polynomial fit.
Statistics: mean, median, mode, standard deviations, and Correlation coefficient, student t-test.

Suggested Readings

1. The chemistry Mathematics Book, E.Steiner, Oxford University Press (2008).
2. Mathematical for Physical Chemistry : F. Daniels, Mc. Graw Hill (1959).
3. Chemical Mathematics D.M. Hirst, Longman (1979).
4. Applied Mathematics for Physical Chemistry, J.R. Barante, Prentice Hall (1974).
5. Basic Mathematics for Chemists, Tebbutt, Wiley (1994).
6. Mathematics for Chemists: Bhupendra Singh, Pragati Prakashan (2013).

Course Title: Computational Methods
Paper Code: CCC.512
Total Hours: 60

L	T	P	Cr
3	1	0	4

Course Objective and Learning Outcomes: This is a fundamental course for students who specialize in Computational Chemistry. The objective of this course is to cover the solution of large scale systems of linear, non-linear and simultaneous equations, matrix and determinants, interpolations, polynomial and spline interpolation, numerical differentiation and integration, curve fitting methods, explicit schemes to solve differential equations, simple optimisation, vectorisation. After, completion of this course will help the students to apply numerical methods to obtain approximate solutions of complex mathematical problems.

Unit I Linear and Non –Linear equations 15 hours
Solution of Algebra and transcendental equations, Bisection, Falsi position and Newton-Rhapson methods-Basic principles-Formulae-algorithms.
Simultaneous equations
Solutions of simultaneous linear equations-Guass elimination and Gauss Seidel iterative methods-Basic principles-
Formulae-Algorithms, Pivotal Condensation.

Unit II 15 hours
Matrix and Determinants:
Matrix Inversion, Eigen-values, Eigen-vector, Diagonalization of Real Symmetric Matrix by Jacobi's Method.

Unit III Interpolations 16 hours

Concept of linear interpolation-Finite differences-Newton's and Lagrange's interpolation formulae-principles and Algorithms

Numerical differentiation and integration:

Numerical differentiation-algorithm for evaluation of first order derivatives using formulae based on Taylor's series, Numerical integration-Trapezoidal Rule, Simpson's 1/3 Rule, Weddle's Rule, Gauss Quadrature Formulae-Algorithms. Error in numerical Integration.

Curve Fit:

least square, straight line and polynomial fits.

Unit IV 14 hours

Numerical Solution of differential Equations: Picards Method, Taylor's Series Method, Euler's Method, Modified Euler's Method, Runge-Kutta Method, Predictor-Corrector Method.

Suggested Readings

1. V. Rajaraman, Computer Oriented Numerical Methods, PHI, 1993.
2. E. Balaguruswamy, Numerical Methods, Tata McGraw Hill, 2017.
3. F.Acton, Numerical Methods that Work, Harper and Row, 1997.
4. S. D. Conte and C.D.Boor, Elementary Numerical Analysis, McGraw Hill, 2005.
5. S. S. Shastri, Introductory Methods of Numerical Analysis, PHI, 2012.

Course Title: Scientific Programming

L	T	P	Cr
3	1	0	4

Paper Code: CCC.508

Total Lectures: 60

Course Objective and Learning Outcomes: The objective of this course is to introduce students to the art of scientific programming. The theory part practical aspects of scientific programming languages Fortran 95/2003 will be taught to students in this course.

Unit I 15 hours

Introduction to Computers and Fortran language

History and evolution of Fortran language, Basic elements of Fortran: Character sets, structure of statements, Structure of a Fortran Program, compiling, linking and executing the Fortran program.

Unit-II 15 hours

Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Unit III 15 hours

Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional

features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types.
Pointers and dynamic data structures- using pointers in assignment statements, with arrays, as components of derived data types and in procedures, Introduction to object oriented programming in Fortran.

Unit IV 15 hours
What is parallel programming, Why use paralle programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting.

Suggested Readings

1. Chapman, Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York (2006).
2. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997).
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press (1996).
4. Parallel Programming in C with MPI and OpenMP by M J Quinn (2003).
5. Introduction to Parallel Computing by Ananth Grama, George Karypis, Vipin Kumar, and Anshul Gupta (2003).

Course Title: Physical Chemistry I
Paper Code: CHM.511
Total Lectures: 54

L	T	P	Cr
3	1	0	4

Course Objective and Learning Outcomes:
The objective of this course is that student learn the thermodynamics, phase transition, fugacity, solid and liquid transitions, and statistical thermodynamics, which are the fundamental branches of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in physical chemistry.

Unit 1 10 hours
Thermodynamics: Thermodynamic functions and their applications, thermodynamic processes, Concepts involved in first, second and third law of thermodynamic, Maxwell relations, Helmholtz and Gibbs Energies, Law of Mass Action, equilibrium constant, Le-Chatlier Principle, temperature-dependence of equilibrium constant and Van't Hoff equation.

Unit 2 10 hours
Partial Molar Properties and Fugacity: Partial molar properties. Chemical potential of a perfect gas, dependence of chemical potential on temperature and pressure, Gibbs- Duhem equation, real gases, fugacity, its importance and determination, standard state for gases.
Phase transition: Phase rule, water, CO2 phase transition, binary and ternary component phase transitions.

Clausius-Clapeyron equation and its application to solid-liquid, liquid-vapour and solid-vapour equilibria.

Unit 3 12 hours

Thermodynamics of Simple Mixtures: Thermodynamic functions for mixing of perfect gases. chemical potential of liquids. Raoult's law, thermodynamic functions for mixing of liquids (ideal solutions only). Real solutions and activities.

Solid-Liquid Solutions: Solutions of nonelectrolytes and electrolytes. Colligative properties of solutions, such as osmotic pressure, depression of the freezing point and elevation of the boiling point.

Unit 4 22 hours

Statistical Thermodynamics: Thermodynamic probability and entropy, Maxwell -Boltzmann, Bose -Einstein and Dermi-Dirac statistics. partition function, molar partition function, thermodynamic properties in term of molecular partition function for diatomic molecules, monoatomic gases, rotational, translational, vibrational and electronic partition functions for diatomic molecules, calculation of equilibrium constants in term of partition function. monoatomic solids, theories of specific heat for solids.

Suggested Readings

1. Barrow, G. M. Physical Chemistry, 5th Edition, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 2-3,5, 5th/3rd Edition, 2011, Macmillan.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9th Edition, 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1st ed., 1998, Viva Books.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3rd edition, 1981, John Wiley and Sons.
6. Engel, T., Reid, P. and Hehre, W. Physical Chemistry, 3rd Edition, 2012, Pearson Education.
7. Rastogi, R. P. and Mishra, R. R. An Introduction to Chemical Thermodynamics 6th ed., 2013, Vikas Publishing
8. Rajaram, J. and Kuriacose, J. C. Chemical Thermodynamics, Classical, Statistical and Irreversible Thermodynamics, 2013, Pearson Education.
9. Laurendeau N. M. Statistical Thermodynamics: Fundamentals and Applications, 2005, Cambridge University Press.
10. Nash, L. K. Elements of Statistical Thermodynamics, 2nd Edition, 2012, Dover Publication Inc.
11. Hill, T. L. An Introduction to Statistical Thermodynamics, 1986, Dover Publications Inc.

Course Title: Scientific Programming Lab (Practical)
Paper Code: CCC.51
Total Lectures: 45

L	T	P	Cr
-	-	6	3

Course Objective and Learning Outcomes:

The objective of this course is to introduce students to the art of scientific programming. The practical aspects of scientific programming languages Fortran and C will be taught to Students in this course.

Unit I 11 hours

Structure of a Fortran Program, compiling, linking and executing the Fortran programs. Constants and variables, assignment statements and arithmetic calculations, intrinsic functions, Program design and branching structures, loop and character manipulation.

Unit II 12 hours

Basic I/O concepts, Formatted READ and WRITE statements, Introduction to Files and File Processing, Introduction to Arrays and procedures, Additional features of arrays and procedures- 2-D and multidimensional arrays, allocatable attays in procedures, derived data types.

Unit III 11 hours

Pointers and dynamic data structures- using pointers in assignment statements, with arrays,as components of derived data types and in procedures, Introduction to object oriented programming in Fortran.
Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination.

Unit IV 11 hours

What is parallel programming, Why use paralle programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting

Suggested Readings

1. Chapman, Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York (2006).
2. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997).
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press (1996).
4. Parallel Programming in C with MPI and OpenMP by M J Quinn
5. Introduction to Parallel Computing by Ananth Grama, George Karypis, Vipin Kumar, and Anshul Gupta.

Course Title: Inorganic Chemistry I
Paper Code: CHM.50
Total Lectures: 54

L	T	P	Cr
3	0	0	3

Course Objective and Learning Outcomes: The objective of this course is that students learn the metal-ligand equilibrium, transition metal complexes, ligand field theory, and crystal field theory, which are the fundamental branches of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in inorganic chemistry.

Unit I 10 hours

Metal-Ligand Equilibria in Solution

Stepwise and overall formation constant and their interaction, trends in stepwise constants, factors affecting the stability of metal complexes with reference to the nature of metal ion and ligand, chelate effect and its thermodynamic origin, determination of binary formation constants by spectrophotometry and potentiometric (pH) methods.

15 hours

Unit 2

Reaction Mechanisms of Transition Metal Complexes

Introduction,potential energy diagram and reactivity of metal complexes, ligand substitution reactions, substitution reactions mechanisms, labile and inert metal complexes, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, anation reaction, substitution reactions in square planar complexes, trans effect, mechanism of the substitution reaction reactions without metal ligand bond cleavage, electron transfer processes outer and inner sphere, Berry pseudorotation.

15 hours

Unit 3

Ligand field theory and molecular orbital theory; nephelauxetic series, structural distortion and lowering of symmetry, electronic, steric and Jahn-Teller effects on energy levels, conformation of chelate ring, structural equilibrium, magnetic properties of transition metal ions and free ions presentive, effects of L-S coupling on magnetic properties, temperature independent paramagnetism(TIP) in terms of crystal field theory CFT and molecular orbital theory (MOT), quenching of orbital angular momentum by crystal fields in complexes in terms of termsplitting. effect of spin-orbit coupling and A, E & T states mixing.

Unit 4 14 hours

Crystal Fields Splitting

Spin-spin, orbital-orbital and spin orbital coupling, LS and J-J coupling schemes, determination of all the spectroscopic terms of p^n, d^n ions, determination of the ground state terms for p^n, d^n, f^n ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, spin orbit coupling parameters (λ) energy separation between different j states, the effect of octahedral and tetrahedral fields on S, P, D and F terms. Splitting patterns of and G, H and I terms. Strong field configurations, transition from weak to strong crystal fields, selection rules of electronic transitions in transition metal complexes, relaxation of the selection rule in centrosymmetric and non-centrosymmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, spectrochemical series, band intensities, factors influencing band widths.

Suggested Readings

1. Cotton, F.A. and Wilkinson G. Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4thedition, 2006, Dorling Kindersley (India) Pvt. Ltd.

3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2ndedition, 2005 (reprinted),Butterworth-
4. Heinemann, A division of Read Educational & Professional Publishing Ltd.
5. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2ndedition, 1984, Elsevier Science Publishers B.V.
6. Carlin, R. L. and Van Duyneveldt, A.J.Magnetic Properties of Transition Metal Compounds, Inorganic
7. Chemistry Concepts 2, SpringerverlagNew York Inc., 1977.
8. Miessler,G. L.andTarr, D. A. Inorganic Chemistry,4thedition, 2011, Pearson Education.
9. Figgis,B.N. Introduction to Ligand Field, 1966Wiley Eastern.
10. Drago,R.S. Physical Method in Chemistry, 1965, W.B. Saunders Company.
11. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5thedition, 2010, Oxford University Press.
12. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
13. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2ndedition, 1993, Affiliated East West Press.
14. Drago, R. S. Physical Methods for Chemists, 2ndedition, 1992, Saunders College Publishing.

Course Title: Organic Chemistry I
Paper Code: CHM.
Total Lectures: 54

L	T	P	Cr
3	0	0	3

Course Objective and Learning Outcomes: The objective of this course is that students learn the reaction mechanism and its intermediates, aromaticity, different sets of aliphatic nucleophilic reaction, aromatic nucliophilic and electrophilic reaction, elimination reaction, addition reaction, which are the fundamental branches of organic chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in computational organic chemistry.

Unit 1 16 hours

Reaction mechanism, structure and reactivity: Types of reaction and mechanisms, kinetic and thermodynamic control, Hammond's postulate, Curtin-Hammett principle, methods of determining mechanisms, isotope effects, effect of structure on reactivity: Hammett equation, Taft equation.

Reactive intermediates: Generation, structure and reactions of carbocations, carbanions, free radicals, carbenes, nitrenes and benzynes. Neighbouring group participation, classical and non-classical carbocations, phenonium ions and norbornyl system.

Aromaticity: Aromaticity in benzenoid and non-benzenoid compounds, antiaromaticity, homoaromatic compounds.

Unit 2 14 hours

Aliphatic nucleophilic substitution reaction: The SN^2, SN^1, mixed SN^2 and SN^1 and SET mechanism, the SN^i

mechanism. nucleophilic substitution at an allylic, aliphatic and vinylic carbon. reactivity effects of substrate structure, attacking nucleophile, leaving group and reaction medium, ambident nucleophile, regioselectivity, competition betweenSN^2 and SN^1 mechanisms.

Aromatic nucleophilic substitution: The SN^{Ar}, bimolecular displacement mechanism and benzyne mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aromatic electrophilic substitution: The arenium ion mechanism, orientation and reactivity, energy profile diagrams, *ortho/para* ratio, *ipso* attack, orientation in other ring systems, quantitative treatment of reactivity in substrates and electrophiles.

Unit 3 12 hours

Elimination reactions: E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, effects of substrate structures, attacking base, the leaving group and the medium, mechanism and orientation in pyrolytic elimination.

Addition to carbon-carbon multiple bonds: Mechanistic and stereochemical aspects of addition reactions involving electrophiles, nucleophiles and free radicals, addition of halogen polar reagents to alkenes, Regio- and chemoselectivity, orientation and reactivity, hydroboration, epoxidation and hydroxylation.

Unit 4 12 hours

Addition to carbon-hetero multiple bonds: Structure and reactivity of carbonyl group towards nucleophilic addition: addition of CN, ROH, RSH, H 2O, hydride ion, ammonia derivatives, LiAlH4, NaBH4, organozinc and organolithium reagents to carbonyl and conjugated carbonyl compounds, Arndt-Eistert synthesis. Mechanism of condensation reactions involving enolates: Aldol, Knoevenagel, Claisen, Dieckmann, Mannich, Benzoin, Perkin and Stobbe reactions. Carboxylic acids and derivatives, hydrolysis of esters and amides, ammonolysis of esters.

Suggested Readings

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2nd ed, 2012, Oxford University Press.
2. Finar, I.L. Organic Chemistry Volume 1, 6th edition, 2012, Pearson Education UK.
3. McMurry J. Organic Chemistry, 8th edition, 2011 Asian Book Pvt. Ltd, New Delhi
4. Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edition, 2013, John Wiley & Sons.
5. Ahluwalia, V. K. and Parashar R. K. Organic Reaction Mechanism, 4th edition, 2011, Narosa Publishing House (P) Ltd., New Delhi.
6. Bansal, R. K. A text book of Organic Chemistry, 5th edition, 2010, New Age International (P) Ltd., New Delhi.
7. Bansal R.K. Organic Reaction Mechanism, 2010, New Age International (P) Ltd., New Delhi.

8. Kalsi, P.S. Organic Reactions and Their Mechanisms. 3rd edition, 2010, New Age International, New Delhi.
9. Kalsi, P.S. Stereochemistry: Conformation and Mechanism, 2010, New Age International Ltd, New Delhi.
10. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3rd edition, 1998, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6th edition, 2011, Prentice- Hall of India, New Delhi.
12. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3rd edition, 2009, Macmillan India Ltd., New Delhi.
13. Robert, J. D. and Casereo, M.C. Basic principle of Organic Chemistry, 2nd edition, 1977, Addison-Wesley.
14. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A.Organic Chemistry. 11th ed., 2013, John Wiley and Sons, Inc.
15. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 6th edition, 1997, Prentice Hall.
16. Eliel, E. L. and Wilen, S. H. Stereochemistry of Organic Compounds, 1994, John Wiley & Sons.

Course Title: Statistics for Chemical and Biochemical Applications
Paper Code: CCC.513
Total Lecture: 45

L	T	P	Cr
3	0	0	3

Course Objective and Learning Outcomes: This course will introduce the basic aspects of various industry based statistical methods to Masters students.

Unit I 11 hours

Overview of Biostatistics: Difference between parametric and non-parametric statistics, Univariant and multivariant analysis, Confidence interval, Errors, Levels of significance, Hypothesis testing.

Unit II 11 hours

Descriptive statistics: Measures of central tendency and dispersal, Histograms, Probability distributions (Binomial, Poisson and Normal), Sampling distribution, Kurtosis and Skewness.

Unit III 11 hours

Experimental design and analysis: Sampling techniques, Sampling theory, Various steps in sampling, collection of data-types and methods.

Unit IV 12 hours

Inferential Statistics: Student's t-test, Paired t-test, Mann-Whitney U-test, Wilcoxon signed-rank, One-way and two-way analysis of variance (ANOVA), Critical difference (CD), Least Significant Difference (LSD), Kruskal– Wallis one-way ANOVA by ranks, Friedman two-way ANOVA by ranks, x2 test. Standard errors of regression coefficients, Comparing two regression lines, Pearson

Product-Moment Correlation Coefficient, Spearman Rank Correlation Coefficient, Power and sampling size in correlation and regression.

Suggested Readings

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley, USA.
2. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc. USA.
3. Norman, G. and Streiner, D. (2008). *Biostatistics: The Bare Essentials.* 3/e (with SPSS). Decker Inc. USA.
4. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*. W.H. Freeman publishers, USA.
5. Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley, USA.

Course Title: Physical Organic Chemistry
Paper Code: CCC.514
Total Lecture: 45

L	T	P	Cr
3	0	0	3

This course on Physical Organic Chemistry will provide conceptual understanding of chemical bonding, aromaticity, structure and stereochemistry, steric and conformational properties, chemical reactivity, correlation of structure with reactivity, Hammond postulates, solvent effects, acidity, nucleophilicity, electrophilicity, studying reaction mechanisms, isotope effects Woodward Hoffmann rules.

Unit-I 11 hours

Chemical bonding: Covalency and molecular structure, approximate molecular orbital theory, properties of covalent bonds, intermolecular forces, aromaticity, structure. Woodward Hoffmann rules.

Unit-II 11 hours

Correlation of structure with reactivity: Electronic demands, the Hammett equation, substituent constants σ, theories of substituent effects, interpretation of σ-values, reaction constants, ρ, deviations from the Hammett equation, dual-parameter correlations, molecular orbital considerations, cross-interaction terms

Unit-III 12 hours

Steric and conformational properties: Origins of steric strain, examples of steric effects upon reactions, measurement of steric effects upon rates.
Solvent effects: structure of liquids, solutions, solvation, thermodynamic measures of solvation, effects of solvation on reaction rates and equilibria, empirical indexes of solvation, use of solvation scales in mechanistic studies.

Unit-IV 11 hours

Kinetic isotope effects: isotopic substitution, theory of isotopic effects, transition-state geometry, secondary kinetic isotope effects, heavy atom isotope effects, tunnel effect
Acids and bases, nucleophiles and electrophiles: acid-base dissociation, the strengths of oxygen and nitrogen acids, linear free-energy relationships, rates of proton transfers, structural effects on amine protonation, factors that

influence carbon acidity, theories of proton transfer, nucleophilicity and electrophilicity and their measurement.

Suggested Readings

1. Neil S. Isaacs, *Physical Organic Chemistry*, 2nd Edition, PHI, 1995.
2. E. V. Anslyn & D. A. Dougherty, *Modern Physical Organic Chemistry*, Illustrated Edition,University Science Books, 2005.
3. Francis A. Carey and Richard J. Sundberg, *Advanced Organic Chemistry*, Part A, Structure and Mechanisms, 5th edition, Springer, 2007.
4. Jerry March, *Advanced Organic Chemistry, Reactions, Mechanims and Structure*, 4th Edition, John-Wiley, 1999.
5. Thomas H. Lowry, Kathleen S. Richardson, *Mechanism and Theory in Organic Chemistry*, 2nd Edition, Harper & Row, 1981.
6. S. P. Gupta, *QSAR and Molecular Modeling*, Anamaya Publishers, 2011.

Course Title: Chemistry without Test Tube (IDE)
Paper Code: CCC.516
Total Hours: 30

L	T	P	Cr
2	0	0	2

Course objective: The aim of this course is to present a qualitative theory of chemical bonding stressing the physical processes which occur on bond formation. Although this is a course in chemistry full of mathematics but, we will use little mathematics to understand the chemical physics behind bonding and reactions.

Unit-I 7 hours

How Science Deals with Complex problems: Level in science, what are molecules made of, interaction between
atoms, simplest examples: H2 and LiH. Thinking in 3D, must we use quantum theory.

Unit-II 8 hours

Electronic Structure: What we know about atoms and molecules; atomic electronic structure, empirical chemistry; what is an orbital (atomic and molecular). Strategy for electronic structure, the Pauli principle and orbitals. Polyatomic Molecules:Methane, electronic structre of methane, shape of the methane molecule, chemist's description of methane.

Unit-III 8 hours

Lone pairs of electrons: Why are Not all electrons involved in bonding? What is a lone pair? Shapes of the simple molecules.
Organic molecules with multiple bonds: Double and triple bonds, ethene and methanal, reactivity of a double bond.
Diatomics with multiple bonds: N2, CO, O2
Dative Bonds: Solvation, reactive lone paire
Delocalized electronic substructures: The benzene molecule, delocalized electrons.

Unit-IV 7 hours

Reactions: What makes a reaction to go? Formation of H2 from H+ and H Formation of lithium borohydride. Nucleophilic, elimination and addition reactions.

Suggested Readings

1. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon,Viva Books, 2011.
2. A. R. Leach, Molecular Modelling Principles and Applications, Prentice Hall (2001).
3. Introduction to Computational Chemistry, F. Jensen, 2nd edition, Wiley-Blackwell (2006).
4. Quantum Chemistry: A Unified Approach, D. B. Cook, 2nd edition, Imperial College Press (2012).
5. Why Chemical Reactions Happen, J. Keeler, P. Wothers, Oxford University Press (2003).
6. Reaction Dynamics, M. Brouard, Oxford Chemistry Primers (1998).

SEMESTER II

Course Title: Quantum Chemistry-I

L	T	P	Cr
3	1	0	4

Paper Code: CCC.526

Total Lecture: 60

Objective and Learning Outcomes: This is a fundamental course for students who specialize in Computational Chemistry. The objective of this course is that students learn the basic concepts of quantum chemistry and apply them to study simple problems that have analytical solutions. In addition, the course will introduce the students towards basic ideas on solving problems in molecular quantum mechanics, which will, in turn, prepare them to take the next advanced level course of Computational Chemistry.

Unit I 16 hours

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian and unitary operators, some important theorems. Schrodinger equation-particle in a box (1D, 3D) and its application, potential energy barrier and tunneling effect, one-dimensional harmonic oscillator and rigid rotor. Angular momentum, eigenvalues of angular momentum operator, Particle in a Ring, Hydrogen Atom.

Unit II 14 hours

Approximate Methods: Perturbation theory for non-degenerate and degenerate states and its applications. The variation theorem and its application.

Unit III 14 hours

Symmetry Point Groups: Determination of point group of a molecule, representations, the great orthogonality theorem, character table, construction

of character tables for c2v and c3v groups, symmetry adapted atomic basis sets, construction of molecular orbitals. The direct product representation.

Unit IV 16 hours

Atomic and Molecular Structure: many electron wave functions, Pauli exclusion principle, Helium atom, atomic term symbols. The self-consistent field method. Slater-type orbitals. Born-Oppenheimer approximation. Molecular orbital treatment for H2+.MO treatment of homo- and hetero nuclear diatomic molecules.Hückel mo treatment of simple and conjugated polyenes and alternate hydrocarbons.

Suggested Readings

1. Quantum Chemistry, I.N. Levine, 5th edition, Pearson Educ., Inc. New Delhi (2000).
2. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon, Viva Books (2011).
3. Valence Theory, J.N. Murrell, S.F.A. Kettle and J. M. Tedder, 2nd edition, John Wiley (1965).
4. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition, Tata Mcgraw Hill (1994).
5. Chemical Applications of Group Theory, F. A. Cotton, John Wiley & Sons (2008).
6. Molecular Symmetry and Group Theory, R. L. Carter, J. Wiley (1998).
7. Group Theory and Chemistry, D. M. Bishop, Dover Publications (1993).
8. Quantum Chemistry, J. P. Lowe, and Peterson, K., Academic Press (2005).

Course Title: Statistical Mechanics I

L	T	P	Cr
3	1	0	4

Paper Code: CCC.524
Total Lectures: 60

Course Objective and Learning Outcomes: The objective of this course is to cover the classical laws of thermodynamics and their application, mathematical review of classical mechanics, postulates of statistical mechanics, Liouville's Theorem, statistical interpretation of thermodynamics, microcanonical, canonical, grant canonical and isobaric-isothermal ensembles, partition function, elementary probability theory, distributions and fluctuations; the methods of statistical mechanics are used to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases; selected topics from low temperature physics and electrical and thermal properties of matter are discussed. After, completion of this course will help the students to apply the principles and techniques from statistical mechanics to a range of modern day research based problems.

Unit I 16 hours

Mathematical Review of Classical Mechanics:

Lagrangian Formulation, Hamiltonian Formulation, Poisson Brackets and Canonical Transformations Classical approach to Ensembles:
Ensembles and Phase Space, Liouville's Theorem, Equilibrium Statistical Mechanics and it's ensembles

Partition Function: Review of rotational, vibrational and translational partition functions. Application of partition functions to specific heat of solids and chemical equilibrium. Real gases.

Unit II 16 hours

Elementary Probability Theory

Distributions and Averages, Cumulants and Fluctuations, The Central Limit Theorem Distributions & Fluctuations:

Theory of Ensembles, Classical and Quantum, Equivalence of Ensembles, Fluctuations of Macroscopic Observable

Unit III 14 hours

Basic Thermodynamics: Review of Concepts, The Laws of Thermodynamics, Legendre Transforms, The Maxwell Relations, The Gibbs-Duhem Equation and Extensive Functions, Intensive Function

Unit IV 14 hours

Bose-Einstein distribution: Einstein condensation. Thermodynamic properties of ideal BE gas.

Fermi-Dirac distribution: Degenerate Fermi gas. Electron in metals. Magnetic susceptibility.

Suggested Readings

1. Statistical Mechanics, by Donald A McQuarrie
2. Introduction to Modern Statistical Mechanics, by David Chandler
3. Statistical Mechanics, by Kerson Haung
4. Statistical Mechanics, by Pathria

Course Title: Physical Chemistry II

Paper Code: CHM.523

Total Lectures: 54

L	T	P	Cr
3	0	0	3

Objective and Learning Outcomes: The objective of this course is that students learn the advanced topics in physical chemistry, eg. electrochemistry, electrochemical cells, reaction kinetics, photochemical process, and adsorption and catalysis, and gain depth knowledge in this fundamental branch of chemistry. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in advanced physical chemistry.

Unit 1 14 hours

Electrochemistry: Ionic equilibria, electrolytic conductance –Kohlrausch's Law, Activity-coefficients, mean activity coefficients; Debye- Huckel treatment of dilute electrolyte solutions, derivation of Debye-Huckel limiting law, extended Debye-Huckel law, and conductometric titrations.

Electrochemical Cells: Nernst equation, redox systems, electrochemical cells, application of electrochemical cell, concentration cells with and without liquid junction, thermodynamics of reversible electrodes and reversible cells, and potentiometric titration.

Unit 2 14 hours

Reaction Kinetics:

Introduction, rates of chemical reactions, complex reactions, steady state approximation,determination of mechanisms of chemical reactions, temperature dependence of rate constant, Arrhenius and Eyring equations and their applications, collision and transition state theories of rate constant, treatment of unimolecular reactions, stearic factor, ionic reactions: salt effect.

Unit 3 14 hours

Photochemical Reactions and Processes: Laws of photochemistry and kinetics of photochemical reactions, measurement of fluorescence and phosphorescence lifetimes and photoinduced electron transfer rates.

Fast Reaction Kinetics: Introduction to time-resolved techniques for absorption and emission measurements, relaxation method, study of kinetics of fast reactions by millisecond stopped-flow, nanosecond flash photolysis techniques, detection and kinetics of reactive intermediates,

Unit 4 12 hours

Adsorption and Catalysis: Colloids and their stability, Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm, Langmuir and Fredulich Isotherms. Homogeneous catalysis and heterogeneous catalysis, enzyme catalysis. Kinetics of catalytic reactions.

Suggested Readings

1. Barrow, G. M. Physical Chemistry, 5th Edition, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 1, 4, 5th Edition, 2011, MACMILLAN Publisher.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 9th Edition, 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1sted., 1998, Viva Books,.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 3rd edition, 1981, John Wiley and Sons.
6. Engel T., Reid, P. and Hehre, W. Physical Chemistry, 3rd Edition, 2012, Pearson Education.
7. Laidler, K. J. Chemical Kinetics, 3rd Edition, 1987, Pearson Education Ltd.
8. Engel T. and Reid, P. Thermodynamics, Statistical Thermodynamics, & Kinetics, 3rd edition, 2013, Pearson Education.
9. Lakowicz, J. R. Principles of Fluorescence Spectroscopy, 3rd edition, 2006, Springer.
10. Raj, G. Surface Chemistry (Adsorption), 4th Edition, 2002, Goel Publishing House.

Course Title: Molecular Spectroscopy
Paper Code: CHM.525
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Objective and Learning Outcomes: This is a fundamental course for students who specialize in Physical/Computational Chemistry. The objective of this course is that students learn the basic concepts of molecular

spectroscopy from a fundamental point of view. The course will help students to understand how spectroscopic transitions come into picture in molecular quantum mechanics.

Unit I 11 hours

Electronic Spectroscopy: Principle of UV-Visible spectroscopy, electronic transition, energy of electronic transition, selection rules, the Franck-Condon principle.

Microwave Spectroscopy: Classification of molecules, rigid rotor model, effect of isotopic substitution on the transition frequencies, intensities, non-rigid rotor, Stark effect, applications.

Unit II 12 hours

Vibrational Spectroscopy: Instrumentation and applications of infrared spectroscopy, simple harmonic oscillator, vibrational energies of diatomic molecules, anharmonicity, vibration-rotation spectroscopy, P, Q, R branches, vibrations of polyatomic molecules, overtones, hot bands and applications.

Raman Spectroscopy - Classical and quantum theories of Raman Effect, pure rotational, vibrational and vibrational-rotational Raman spectra, mutual exclusion principle, resonance Raman Spectroscopy, surface enhanced Raman spectroscopy, coherent anti stokes Raman spectroscopy.

Unit III 12 hours

Nuclear Magnetic Resonance (NMR) Spectroscopy: Basic principles, instrumentation, magnetization vector and relaxation, NMR transitions, Bloch equation, relaxation effects and mechanism, double resonance and spin tickling, effect of quadrapole nuclei, nuclear overhauser effect (NOE), multiple pulse methods, NMR in medical diagnostics.

Unit IV 10 hours

Lasers and Laser Spectroscopy: Principles of laser action, pulsed lasers, examples of lasers: He-Ne, Nd-YAG, dye lasers.

Suggested Readings

1. Modern Spectroscopy, J. M. Hollas, 4th edition, John Wiley & Sons, Ltd. (2004).
2. Introduction to Molecular Spectroscopy, G. M. Barrow, McGraw-Hill (1962).
3. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E.M. Mc Cash, 4th edition, Tata McGraw Hill, New Delhi (1994).
4. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, 3rd Edition, Springer.
5. Introduction to Magnetic Resonance A. Carrington and A. D. Mc Lachlan, Chapman and Hall, London (1979).
6. Nuclear Magnetic Resonance Spectroscopy, R. K. Harris, Addison Wesley, Longman Ltd, London (1986).

Course Title: Physical Chemistry II
Paper Code: CCC.527
Total Hours: 60

L	T	P	Cr
0	0	4	2

Objective and Learning Outcomes: The objective of this course is that student's get an in hand experience of experimental physical chemistry. This experience will help the students better appreciate how the experimental information gained in Chemistry can be enhanced with the help of Computational Modeling techniques that they will learn in subsequent semester of the programme.

1. Determination of strength of a given base by titrating with an acid conductometrically.
2. Determination of solubility and solubility product of sparingly soluble salts (e.g., PbSO4, BaSO4) conductometrically.
3. Determination standard electrode potential of Fe^{2+}/Fe^{3+} system by potentiometer using potassium permanganate solution.
4. Determination of pKa of acetic acid and glycine by pH meter using NaOH.
5. Determination of relative and absolute viscosity of a given liquid.
6. Determination of surface tension of alcohols.
7. Determination of refractive indices (RI) of given liquids and determination of the concentration from RI.
8. Determination of concentrations of proteins and DNA using spectrophotometer
9. Preparation of buffers and measurement of their pH.
10. Verification of the Lambert Beer's law.
11. Structural analysis of amino acids and proteins using CD and Fluorescence spectrometer.
11. Study of chemical and thermal denaturation (Tm and Hm) of proteins and DNA using UV-Visible and CD spectrometer.
12. Molecular weight of a non-electrolyte by cryoscopy method.
13. Determination of stability constant of Fe(III)-salicyclic acid complex by spectrophotometer.
14. Determination of mean, median, standard errors, standard deviation, coefficient of variance using software.

Suggested Readings

1. Nad, A. K., Mahapatra, B. and Ghoshal, A. An Advanced Course in Practical Chemistry, 2014, New Central Book Agency (P) Ltd.
2. Maity S. and Ghosh, N. Physical Chemistry Practical, 2012, New Central Book Agency (P) Ltd.
3. Elias, A. J. Collection of Interesting General Chemistry Experiments, 2008, Universities Press.
4. Khosla, B.D., Garg, V.C., and Gulati A.R., Senior Practical Physical Chemistry, 2007, S. Chand& Sons.
5. Yadav, J.B. Advanced Practical Physical Chemistry, 2008, Krishna Prakasan Media.
6. Das, R.C. and Behra, B. Experimental Physical Chemistry, 1983, Tata McGraw-Hill.
7. James, A.M. and Prichard, F.E. Practical Physical Chemistry, 3rdedition, 1974, Longman, Harlow.
8. Ghosh, J.C., Experiments in Physical Chemistry, 1990, Bharati Bhavan.

Course Title: Computational Methods Lab (Practical)
Paper Code: CCC.528
Total Hours: 90

L	T	P	Cr
0	0	6	3

Course Objective and Learning Outcomes: The purpose in this course is to cover the solution of transcendental and polynomial equations, linear curve fitting, matrix and determinants, differentiation and integration, explicit schemes to solve differential equations, and simple optimisation. After, completion of this course will help the students to write computer code of various numerical methods in a modern computer language.

Unit I 22 hours

MATLAB:

Basics of Mat lab- Mat lab windows – On-line help- Input- Output-File types- Platform Dependence -Creating and working with Arrays of Numbers – Creating, saving, plots printing Matrices and Vectors – Input – Indexing – matrix Manipulation-Creating Vectors Matrix and Array Operations Arithmetic operations-Relational operations – Logical Operations – Elementary math functions, Matrix functions – Character Strings Applications.

Unit II Application: 23 hours

Jacobi Method of Matrix Diagonalization, Solution of transcendental or polynomial equations by the Newton Raphson method, Linear curve fitting and calculation of linear correlation coefficient, Matrix summation, subtraction and multiplication, Matrix inversion and solution of simultaneous equation, Gaussian elimination, Finding Eigen values and eigenvectors, Matrix factorizations Curve Fitting – Polynomial curve fitting on the fly, Least squares curve fitting, General nonlinear fits, Lagrange interpolation based on given input data, Numerical integration using the Simpson's method, Numerical integrationg using the Gaussian quadrature method, Solution of first order differential equations using the Rung-Kutta method, Numerical first order differentiation of a given function, Fast Fourier Transform, Monte Carlo integration.

Suggested Readings

1. Y.Kirani Singh and B.B.Chaudhuri, MATLAB Programming, Prentice-Hall India, 2007
2. Rudra Pratap, Getting Started with Matlab 7, Oxford, Indian University Edition, 2006
3. Numerical Methods, E. Balaguruswamy, Tata McGraw Hill
4. Computer oriented numerical methods-Rajaraman

Course Title: Seminar -I
Paper Code: CCC.542

L	T	P	Cr
0	0	2	1

The objective of this course would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.

The evaluation criteria shall be as follows:		
S.No.	Criteria	Marks
1	Content	10
2	Presentation Skills	10
3	Handling of queries	05

Course Title: Inorganic Chemistry II
Paper Code: CCC.521
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Objective and Learning Outcomes: The objective of this course is that students learn the advanced topics in inorganic chemistry, eg symmetry operation and group theory, metal complexes, inorganic rings and cages. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in inorganic chemistry.

Unit 1 12 hours

Symmetry

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination, 12 hours

Unit 2

Group theory

Determination of reducible and irreducible representations, character tables, construction of character tables for C2v, C3v, use of symmetry in obtaining symmetry of orbitals in molecules.

Unit 3 14 hours

Metal Complexes

Organic-transition metal chemistry, complexes with π-acceptor and σ-donor ligands, 18-electron and 16-electron rules, isolobal analogy, structure and bonding. Metal carbonyls, structure and bonding, vibrational spectra of metal carbonyls for bonding and structure elucidation, important reaction of metal carbonyls. Preparation, bonding structure and important reactions of transition metal nitrosyl, dinitrogen and dioxygencomplexes, tertiary phosphine as ligand. Metallocenes, metal cluster compounds, metal-metal bond, carbonyl and non-carbonyl clusters, fluxional molecules.

Unit4 16 hours

Inorganic chains, rings and cages

a) Chains: Catenation, heterocatenation, isopolyanions and heteropolyanions.

b) Rings: Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic inorganic systems.

c) Cages: Cage compounds having phosphours, oxygen, nitrogen and sulphur: boron cage compounds, boranes, carboranes and metallocenecarboranes.

Suggested Readings

1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 6th edition, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 4th edition, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2nd edition, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2nd edition, 1984, Elsevier Science Publishers B.V.
5. Carlin, R. L. and Van Duyneveldt, A.J. Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springerverlag New York Inc., 1977.
6. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5th edition, 2010, Oxford University Press.
7. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
8. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2nd edition, 1993, Affiliated East West Press.
9. Drago, Russell S. Physical Methods for Chemists, 2nd edition, 1992, Saunders College Publishing

Course Title: Organic Chemistry II
Paper Code: CCC.522
Total Lectures: 45

L	T	P	Cr
3	0	0	3

Objective and Learning Outcomes: The objective of this course is that students learn the advanced topics in organic chemistry eg. stereochemistry, photochemistry, pericyclic and cycloaddition reaction, sigmatropic rearrangements. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in advanced organic reactions.

Unit 1 12 hours

Stereochemistry: Elements of symmetry, chirality, projection formulae, configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, D/L, R/S, *E*/*Z* and *cis*/*trans* configurational notations, *threo* and *erythro* isomers, methods of resolution, optical purity, 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, conformational analysis of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives, decalins, 1,2, 1,3- , 1,4-disubstituted cyclohexane derivatives and D-Glucose, effect of conformation on reactivity, conformation of sugars.

Unit 2 12 hours

Photochemistry: Jablonski diagram, singlet and triplet states, photosensitization, quantum efficiency, photochemistry of carbonyl compounds, Norrish type-I and type-II cleavages, Paterno-Buchi reaction, Photoreduction, Di π – methane rearrangement.

Photochemistry of aromatic compounds, Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction, Singlet molecular oxygen reactions.

Unit 3 16 hours

Pericyclic chemistry:

Introduction, Phases, nodes and symmetry properties of molecular orbitals in ethylene, 1,3-butadiene, 1,3,5-hexatriene, allyl cation, allyl radical, pentadienyl cation and pentadienyl radical.

Electrocyclic reactions: Conrotation and disrotation, 4n and 4n+2 systems. Woodward-Hoffmann rules. (i) Symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and correlation diagrams.

Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions and stereochemical aspects. Diels-Alder reaction. Woodward-Hoffmann Selection rules. Explanation for the mechanism by (i) Conservation of orbital symmetry and correlation diagrams (ii) FMO theory

Sigmatropic reactions: [1,j] and [i,j] shifts; suprafacial and antarafacial, selection rules for [l, j] shifts; Cope and Claisen rearrangements; explanation for the mechanism by (i) symmetry properties of HOMO (ii) Introduction to cheletropic reactions and the explanation of mechanism by FMO theory.

Unit 4 14 hours

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Benzil-Benzillic acid, Favorskii, Neber, Beckmann, Hofmann, Curtius, Schmidt, Carroll, Claisen, Cope, Gabriel–Colman, Smiles and Sommelet–Hauser rearrangements.

Selective Name Reactions: Ene/Alder-ene reaction, Dakin reaction, Reformatsky, Robinson annulation, Michael addition, Hofmann-Loffler Fretag, Chichibabin reaction.

Suggested Readings

1. Acheson, R.M. An introduction to the Chemistry of Heterocyclic Compounds, 3rd ed, 1976 Wiley India Pvt. Ltd.
2. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2nd ed, 2012, Oxford University Press.
3. Ahluwalia, V. K. and Parasar R. K. Organic Reaction Mechanism, 4th ed, 2011, Narosa Publishing House (P) Ltd., New Delhi.
4. Bansal, R. K. A Textbook of Organic Chemistry, 5th edition, 2010, New Age International (P) Ltd., New Delhi.
5. Bansal R.K. Organic Reaction Mechanism,2010, New Age International (P) Ltd., New Delhi.

6. Bansal, R.K. Hetrocyclic Chemistry, 5th edition, 2010, New Age International (P) Ltd., New Delhi.
7. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part A, 4th ed, 2002, Kluwer Academic Publishers.
8. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part B, 5th ed, 2007, Springer Science and Business Media Ltd.
9. Finar, I.L. Organic Chemistry Volume 1, 6th edition, 2012, Pearson Education UK.
10. Gilchrist, T.L. (1997). Heterocyclic Chemistry, 3rd edition, 1997, Addison Wesley Longman Publishers, US.
11. Gupta R.R., Kumar M. and Gupta V. Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3, 2010, Springer Verlag, India.
12. Joule, J.A. and Mills, K. Heterocyc1ic Chemistry, 5th edition,2010, Blackwell Publishers, New York.
13. Kalsi, P.S. Organic Reactions and Their Mechanisms. 3rd edition, 2010, New Age International, New Delhi.
14. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 3rd edition, 1998, Addison-Wesley Longman Inc., New York.
15. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 6th edition, 2011, Prentice- Hall of India, New Delhi.
16. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 3rd edition, 2009, Macmillan India Ltd., New Delhi.
17. Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin V. V. Handbook of Heterocyclic Chemistry, 3rd edition, 2010, Elsevier UK.
18. Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 7th Edition, 2013, John Wiley & Sons.
19. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 6th edition, 1997, Prentice Hall.
20. Norman, R.O.C. and Coxon, J.M. Principles of Organic Synthesis, 3rd edition, 1998, Nelson Thornes, Blackie Academic & Professional.

Course Title: Density Functional Theory
Paper Code: CCC.529, Credits: 3
Total Lecture: 45

Objective and Learning Outcomes: This is a specialization course for students of Computational Chemistry. The objective of this course is to make the students understand the basics of Density Functional Theory (DFT), which is a popular electronic structure method. With the increasing power of computers, DFT-based calculations are emerging as a useful tool to characterize the properties of molecules and materials. This course will review the various theories/approximations necessary to understand most popular framework of modern DFT.

Unit-I 12 hours

Many-body Approximations: Schrodinger equation and its solution for one electron and two electron systems, Hamiltonian of many particles system, Born-Oppenheimer approximation, Hartree theory, Idea of self consistency, Exchange energy and interpretation, Identical particles and spin, Hartree-Fock theory,

Antisymmetric wavefunctions and Slater determinant, Koopmans' theorem, Failures of Hartree-Fock in solid state, Correlation energy, Variational principle, Connection between Quantum Mechanics,Variational Principle and Classical Mechanics.

Unit-II 11 hours

From Wave Functions to Density Functional: Idea of functional, Functional derivatives, Electron density, Thomos Fermi model, Hohenberg-Kohn theorems, Approximations for exchange-correlation: Local density approximation (LDA) and local spin density approximation (LSDA), Gradient expansion and generalized gradient approximation (GGA), Hybrid functionals and meta-GGA approaches. Self-interaction corrections (SIC).

Unit-III 11 hours

Practical Implementation of Density Functional Theory (DFT): Kohn-Sham formulation: Plane waves and pseudopotentials, Janak's theorem, Ionization potential theorem, Self consistent field (SCF) methods, Understanding why LDA works, Consequence of discontinuous change in chemical potential for exchange-correlation, Strengths and weaknesses of DFT.

Unit-IV 11 hours

Electronic Structure with DFT: Free electron theory, Band theory of solids, Tight-binding method, Semiconductors, Band structure, Density of states. Interpretation of Kohn-Sham eigenvalues in relation with ionization potential, Fermi surface and band gap.

Suggested Readings

1. Richard M. Martin, Electronic Structure: Basic Theory and Practical Methods, (Cambridge University Press, 2004)
2. Robert G. Parr and Weitao Yang, *Density Functional Theory of Atoms and Molecules*, (Oxford University Press, 1994).
3. David S. Sholl and Janice A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).
4. June Gunn Lee, *Computational Materials Science: An Introduction*, (CRC Press 2011)
5. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007

Course Title: Introduction to Quantum Dynamics
Paper Code: CCC.530
Total Lecture: 45

L	T	P	Cr
3	0	0	3

Course Objective and Learning Outcomes: This course will introduce the basic aspects of time dependent quantum wavepacket dynamics to Masters students.

Unit I 12 hours

Separation of electronic and nuclear motions: adiabatic representation, Born-Oppenheimer approximation, Hellmann-Feynman theory, diabatic representation, transformation between two representations, crossing of adiabatic potentials.

TDSE: separation of variables and reconstitution of the wavepacket, expectation values, free-particle wavepacket:
centre and dispersion of the wavepacket.

Unit II 11 hours

Gaussian wavepacket: Gaussian free particle, general properties of Gaussian wavepackets, Gaussian in a quadratic
potential. Correspondence between Classical and Quantum Dynamics: Ehrenfest's Theorem, Bohmian Mechanics and the Classical limit.

Unit III 11 hours

Spectra as Fourier transforms of wavepacket correlation functions. 1D barrier scattering: wavepacket formulation of reflection and transmission coefficients, cross-correlation function and S-matrix.

Unit IV 11 hours

Numerical methods for solving the TDSE: spectral projection and collocation, pseudospectral basis, gaussian quadrature, represntation of the hamiltonian in the reduced space, discrete variable representation, Fourier method, time propagation.

Suggested Readings

1. D. J. Tannor, *Introduction to Quantum Mechanics: A Time-dependent Perspective*, University Science Books, 2006.
2. Edited by R E Wyatt and J Z H Zhang, *Dynamics of Molecules and Chemical Reactions*, CRC Press, 1996.
3. K. C. Kulander, *Time-dependent Methods for Quantum Dynamics*, Elsevier Science, 1991.
4. J. Z. H. Zhang, *Theory and application of Quantum Molecualr Dynamics*, World Scientific Publishing Company, 1998.
5. Edited by M Brouard and C Vallance, *Tutorials in Molecular Reaction Dynamics,* Royal Society of Chemistry, 2010.
6. Edited by D. A. Micha, I. Burghardt, *Quantum Dynamics of Complex Molecular Systems*, Springer-Verlag, 2006.

SEMESTER III

Course Title: Electronic Structure Theory
Paper Code: CCC.556
Total Hours: 60

L	T	P	Cr
3	1	0	4

Objective and Learning Outcomes: This is an advanced course for students who specialize in Computational Chemistry. The objective of this course is that students learn the techniques of molecular quantum chemistry (eg. Hartree-Fock SCF and Roothaan-Hartree-Fock method, CI Interaction, CCSD, CCSD(T), Kohn-Sham equations) and apply them to study chemical and biochemical problems.

Unit I 16 hours

Review of molecular structure calculations, Hartree-Fock SCF method for molecules

Unit II 15 hours

Roothaan-Hartree-Fock method, selection of basis sets.

Unit III 14 hours

Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster Method.

Unit IV 15 hours

Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR.

Suggested Readings

1. Introduction to Computational Chemistry, F. Jensen, 2nd edition, Wiley-Blackwell (2006).
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, 3rd ed, OUP, Oxford (1997).
3. Quantum Chemistry, H. Eyring, J. Walter and G.E. Kimball, (1944) John Wiley, New York.
4. Quantum Chemistry, I.N. Levine, 5th edition (2000), Pearson Educ., Inc., New Delhi.
5. Modern Quantum Chemistry: Introduction to Advanced Electronic Structure, A. Szabo and N. S. Ostlund, (1982), Dover, New York.

Course Title: Fundamentals of Molecular Simulations

L	T	P	Cr
4	0	0	4

Paper Code: CCC.554

Total Lecture: 60

Course Objective and Learning outcomes: The objective of this subject is to ensure that a student learns modelling of molecular structures and understanding the dynamics of the structural transitions, which will help them use the techniques of molecular simulations in their further potential careers in academia and industry.

Unit I 15 hours

Molecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example.

Force Fields and Molecular Representation – (a) Intramolecular Interactions, (b) Non-bonded Interactions – London (van der Waals) Interactions, Electrostatic Interactions, (c) Hydrogen Bonds, (d) Constraints and Restraints,

(e) United Atom and Other Coarse-Grained Approaches, (f) Non-pairwise Interactions, (g) How accurate are force fields?

Example: Protein, Nucleic Acid, Small Molecule Force Field, Water Models.

Unit II 15 hours

Methods for Simulating Large Systems

(a) Non-bonded Cutoffs – Shifted Potential and Shifted Force, Switching Functions, Neighbor Lists, (b) Boundaries

– Periodic Boundary Conditions, Stochastic Forces at Spherical Boundary, (c) Long-range Interactions – The Ewald Sum, The Reaction Field Method

Unit III 15 hours

Energy Minimization and Related Analysis Techniques

(a) Steepest Descent, (b) Conjugate Gradient, (c) Newton-Raphson, (d) Comparison of Methods, (e) Advanced Techniques: Simulated Annealing, Branch-and-bound, Simplex, (f) What's the big deal about the minimum? Introduction to Equilibrium Statistical Mechanics

(a) Phase space, Ergodicity, and Liouville's theorem, (b) Ensemble theory, Thermodynamic averages - Microcanonical Ensemble, Canonical Ensemble, Other MD Simulation Related Ensembles (c) Statistical Mechanics of Fluids

Unit IV 15 hours

Simulation Methods:

Monte Carlo: (a) MC integration and Markov chains, (b) The Metropolis method, (c) Biased MC

Molecular Dynamics: (a) Classical Mechanics: Equations of Motion, (b) Finite Difference Methods: Verlet

Algorithm, Velocity Verlet, The Time Step: Practical Issues, Multiple time-step algorithms (c) Constraint

Dynamics: Fundamental concepts, SHAKE and RATTLE, (d) Temperature: Maxwell-Boltzmann distribution of

velocities, (e) Temperature Control: Velocity Scaling, Andersen's Method, Nose-Hoover Dynamics, (f) Pressure

Control: Andersen's Method, Nose-Hoover Method, Rahman-Perrinilo Method, (g) Calculating properties from MD trajectories, (h) Hybrid MC,

Free Energy: (a) Perturbation Methods, (b) TI (Thermodynamic Integration) Brownian dynamics and the Langevin Equation.

Suggested Readings

1. Computer Simulation of Liquids, by M.P. Allen and D.J. Tildesley, (QC 145.2.A43 1992)
2. Understanding molecular simulation, by Daan Frenkel and Berend Smit, (QD 461 .F86 1996)
3. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.

Course Title: Molecular Simulations Lab (Practical)

Paper Code: CCC.555

L	T	P	Cr
0	0	6	3

Total Lecture: 90

Course Objective and Learning outcomes: The objective of this subject is to ensure that a student gains practical in-hand experience of various modeling and classical simulation tools, including, but not limited those that are used in macromolecular modeling. The course will help the students learn the use the techniques of molecular simulations, which will enhance their employability in their further potential carrers in academia and industry.

1. Linux basics and remote computing
2. Coordinate generations and inter-conversions of small molecules
3. Energy minimizations and optimization, *ab initio methods*
4. Advanced Visualization Software and 3D representations with VMD
5. Introduction to PDB Data
6. Secondary Structure Prediction, Fold Recognition

7. Molecular Dynamics with GROMACS
    a. Water liquid structure and dynamics
    b. Simulation of Ionic Solutions
    c. Simulation of Protein in Water
    d. Simulation of Membrane Proteins
    e. Simulations of DNA
8. Review of Molecular Dynamics Principles

Suggested Readings

1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach",(2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

Course Title: Bio-inorganic and Biophysical Chemistry
Paper Code: CHM.553
Total Contact Hours: 45

L	T	P	Cr
3	0	0	3

Learning objective and outcomes: To provide knowledge of structure, function, and physicochemical properties of biomolecules. The students will acquire knowledge of structure and biological functions of proteins and enzymes and the role of metals in biology.

Unit 1 11 hours

Inorganic Chemistry of Enzymes - I

Metalloporphyrins: Hemoglobin and myoglobin, nature of heme-dioxygen binding, model systems, cooperativity in hemoglobin, physiology of myoglobin and hemoglobin, structure and function of haemoglobin and myoglobin. Other iron-prophyrin biomolecules, peroxidases and catalases, cytochromes, cytochrome P450 enzymes, other natural oxygen carriers, hemerythrins, electron transfer. Biochemistry of iron, iron storage and transport, ferritin, transferrin, bacterial iron transport.

Unit 2 11 hours

Inorganic Chemistry of Enzymes - II

Metallothioneins: Ferridoxins, carboxypeptidase, carbonic anhydrase, blue copper proteins, superoxide dismutase, hemocyanines, photosynthesis, respiration and photosynthesis; chlorophyll and photosynthetic reaction center.

Enzymes: Structure and function, inhibition and poisoning vitamin B12 and B12 coenzymes metallothioneins, nitrogen fixation, in-vitro and in-vivo nitrogen fixation, bio-inorganic chemistry of Mo and W.

Unit 3 11 hours

Metal Ions in Biological Systems

Role of metal ions in replication and transcription process of nucleic acids. Biochemistry of calcium as hormonal messenger, muscle contraction blood clotting, neurotransmitter, metals in the regulation of biochemical events.

Metal complexes for therapeutic uses (cisplatin, carboplatin, non platinum metal complexes).

Unit 4 12 hours

Biophysical Chemistry

Principles of biophysical chemistry (pH, buffer, reaction kinetics, thermodynamics), structure and physical properties of amino acids, physical principle of structure, function, and folding of proteins, conformations of proteins (Ramachandran plot, secondary, tertiary and quaternary structure; domains; motif and folds), determination of protein structures by spectroscopic methods (CD, FTIR, NMR), thermodynamics of protein folding by spectroscopic and calorimetric methods, ultrafast folding dynamics study by laser flash photolysis, protein conformational study by NMR and fluorescence spectroscopy, measurement of hydrodynamic radii by dynamic light scatter

Suggested Readings

1. Huheey, J. E.,Keiter,E. A. AndKeiter, R.L. Inorganic Chemistry Principles of Structure and Reactivity, 4th edition, 2006, Haper Collins.
2. Douglas, B., McDaniel,D. AndAlexander, J. Concepts and Models of Inorganic Chemistry, 3rd edition, 2006, John Wiley and Sons.
3. Cotton, F.A. andWilkinson, G. Advanced Inorganic Chemistry: A Comprehensive Text, John Wiley, 5th ed.
4. Elschenbroich,Ch. and Salzer,A. Organometallics. A Concise Introduction, 2nd edition, 1992, Wiley-VCH.
5. Atkins, P., Overtone, T., Rourke, J., Weller, J. And Armstrong, F. Shriver and Atkin'sInorganic Chemistry, 5thedition, 2010, OUP.
6. Cowan, J.A. Inorganic Biochemistry: An Introduction, 2nd edition, 1997, Wiley – VCH,.
7. Lippard,S. J. Progress in Inorganic Chemistry,Vols. 18, 1991, Wiley-Interscience.
8. Lippard,S. J. Progress in Inorganic Chemistry,Vols. 38, 1991, Wiley-Interscience.
9. Lesk, A.M., Introduction to Protein Science: Architecture, Function, and Genomics, 2nd ed, 2010, OUP.
10. Cantor, C.R. and Schimmel, P.R., Biophysical Chemistry, 1980, Freeman.
11. Van Holde, K.E., Johnson, W.C. and Ho, P.S., Principles of Physical Biochemistry, 2nd ed, 2006, Pearson Education.
12. Harding, S.E. and Chowdhry, B. Z. Protein-Ligand Interactions, 2001, Oxford University Press.

Course Title: M.Sc. Project work I

L	T	P	Cr
0	0	12	6

Paper Code: CCC.599

Course Objective and Learning Outcomes: The objective of dissertation part I would be to ensure that the student learns the nuances of the scientific

research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

The Evaluation criteria shall be multifaceted as detailed below:

S.No.	Criteria	Marks allotted
Theoretical work		
1.	Review of literature and Bibliography	25
2.	Identification of gaps in knowledge	15
3.	Objective formulation	15
4.	Methodology	35
5.	Presentation	35
Experimental Work		
6.	Continuous evaluation by guide	25
	Total	150

The final presentation shall be evaluated by a three membered committee consisting of

a. HOD/OHOD of the department
b. Another teacher from allied department
c. Supervisor (and Co-supervisor if applicable)

Of as recommended by School Board.

SEMESTER IV

Course Title: Credit Seminar -II
Paper Code: CCC.544

L	T	P	Cr
0	0	2	1

The objective of this course would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.
The evaluation criteria shall be as follows:

S.No.	Criteria	Marks
1	Content	10
2	Presentation Skills	10
3	Handling of queries	05

Course Title: M.Sc. Project work II
Paper Code: CCC.599

L	T	P	Cr
0	0	12	6

Course Objective and Learning Outcomes: The objective of dissertation part II would be to ensure that the student learns the nuances of the scientific research. Herein the student shall have to carry out the experiments to achieve the objectives as mentioned in the synopsis. The data collected as a result of experiments must be meticulously analyzed in light of established scientific knowledge to arrive at cogent conclusions.

The Evaluation criteria shall be multifaceted as detailed below:

		Total marks 150*
S.No.	Criteria	Marks allotted
1.	Report Writing	50
2.	Presentation and defense of research work	50
3.	Continuous evaluation of student by Guide	50
	Total	150

The final presentation shall be evaluated by a three membered committee consisting of a. HOD / OHOD of the department
b. Another teacher from allied department
c. Supervisor (and Co-supervisor if applicable)
*of as recommended by Schol Board.

Course Title: Biomolecular Modeling Lab (Practical)
Paper Code: CCC.571
Total Hours: 90

L	T	P	Cr
0	0	6	3

Course Objective and Learning Outcomes: The objective of this subject is to ensure that a student learns practical aspects of modelling of biomolecular structures.

1. Introduction to protein structure prediction
2. Homology or comparative modeling using MODELLER
3. Effect of sequence on model accuracy (eg. FABP)
   a. Select template structures
   b. How to validate protein structure
   c. Validate homology model and compare with x-ray structure
4. Homology Modeling and MD Refinement
5. Molecular Recognition
   a. Prediction of Protein-ligand interaction sites
   b. Prediction of Protein-nucleic acid interaction sites
   c. Prediction of Protein-protein interaction sites
6. Structure based Drug Designing
   a. Molecular Docking
   b. De Novo Ligand Design
   c. Virtual Screening

   Ligand based Drug Design
   a. Pharmacophore Identification
   b. QSAR
7. Special Topic: (a) Umbrella Sampling
   (b) Free Energy Calculations
   (c)Multicomponent Systems

Suggested Readings

1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. “Combinatorial Chemistry – A practical approach”,(2000) Oxford University Press, UK.

3. Lednicer, D. “Strategies for Organic Drug Discovery Synthesis and Design”; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F “Combinatorial chemistry and molecular diversity in drug discovery” (1998) Wiley-Liss Publishers.

Course Title: Electronic Structure Theory Lab (Practical)
Paper Code: CCC.572
Total Hours: 90

L	T	P	Cr
0	0	6	3

Course Objective and Learning Outcomes: This course will provide practical experience to the students through use of important Computational Chemistry softwares. Following experiments will be carried out in the lab.

1. Introduction to Gaussian calculations.
2. Carrying of conformational analysis of small molecules using G09.
3. Vibrational spectra, NMR spectra and TDDFT calculations using G09.
4. Modeling chemical reactions including transition state calculations.
5. 2D potential energy suface generation for two torsion angles.
6. Pseudopotential generation and testing of Si atom.
7. Functional and basis set dependent lattice constant and bulk modulus of Fe solid.
8. Total energy versus cell size and binding energy of H2 and H2O molecules.
9. Density of states and electronic band structure of bulk Si.
10. To study the structural and electronic properties of graphene and its nanoribbon.
11. Building macromolecules, extracting crystal structure/NMR coordinates and generating models for MD simulations. RESP charge calculation.
12. Energy minimization during MD simulations- Steepest descent and conjugate gradient methods.
13. Gas phase MD simulations.
14. MD simulations in implicit solvent.
15. MD simulations in Explicit solvents.

References

1.David S. Sholl and Janice A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).
2. http://departments.icmab.es/leem/siesta/Documentation/Manuals/manuals.html
3.http://blogs.cimav.edu.mx/daniel.glossman/data/files/Libros/Exploring%20Chemistry%20With%20Electronic %20Structure%20Methods.pdf
http://ambermd.org/tutorials/

Course Title: Biomolecular Modeling
Paper Code: CCC.573
Total Lectures: 60

L	T	P	Cr
4	0	0	4

Course Objective and Learning outcomes: The objective of this subject is to ensure that a student learns advanced modelling techniques for molecular modeling and understanding the dynamics of the structural transitions, which will help them to use those advanced modeling techniques further in their potential careers in academia and industry.

Unit I 15 hours

Introduction: What is Biomolecular Modeling and the importance of Biomolecular Simulation. Principles of protein and nuclic acid structure: Tertiary structure, Qaternary structure, Similarity of ternary and quaternary structure

Protein secondary structure: Introduction, Hydrogen bond, Defining a secondary structure element, Methods for predicting secondary structure

Experimental methods for protein structure determination: X-ray crystallography, Nuclear magnetic resonance (NMR)

Unit II 15 hours

Basic concepts: Units and derivatives, Force field and energy landscape, Truncation of nonbonded interactions

Conformational Sampling: Minimization and alogrithms, Molecular dynamics, Ensembles (statistical mechanics), Monte Carlo simulations

Solvation: Periodic boundary condition, Ewald summation, Implicit solvent model and continuum electrostatics, Monte Carlo simulation on parallel computers

Advanced Techniques: Replica-exchange molecular dynamics, Restraint potentials, Free energy calculations, Membrane simulations

Unit III 15 hours

Protein tertiary structure modeling: Basic concepts, Protein folding and dynamic simulation, Modeling protein sidechains, Comparative modeling, Threading, Ab initio modeling, Combined modeling approaches, CASP: A blind protein structure prediction competition

Introduction to protein design: "Rational" design efforts, Experimental methods (directed evolution), Computational protein design

Unit IV 15 hours

Protein Interaction

Protein quaternary structure modeling: Basic concepts, Energy landscapes, Docking algorithms – foundation, Docking algorithms – current & future, Docking example, CAPRI, Protein Structure Initiative, Computational proteomics

Designing protein-protein interfaces: Designing for affinity, Designing for specificity

Suggested Readings

1. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
2. Fenniri, H. "Combinatorial Chemistry – A practical approach",(2000) Oxford University Press, UK.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
4. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

Course Title: Seminar -II
Paper Code: CCC.544

L	T	P	Cr
0	0	2	1

The objective of this course would be to ensure that the student learns the aspects of the seminar presentation. Herein, the student shall have to present a selective overview of a scientific problem with focus of literatural knowledge.

The evaluation criteria shall be as follows:

S.No.	Criteria	Marks
1	Content	10
2	Presentation Skills	10
3	Handling of queries	05

L	T	P	Cr
0	2	0	2

Course Title: Enrich Chemistry Course-I
Paper Code: CCC.577
Semester: IV
Course: CF

Curse Objective: Past Question papers would be discussed / given to the students for preparation

Mode of Transaction

7. Self-learning, Inquiry training, Group discussion, Co operative learning, Problem solving

Evaluation Criteria

As per UGC guidelines on adoption of CBCS

Semester: IV

L	T	P	Cr
0	2	0	2

Course Title: Enrich Chemistry Course-II
Paper Code: CCC.578
Course: CF

Curse Objective: Past Question papers would be discussed / given to the students for preparation

Mode of Transaction

Self-learning, Inquiry training, Group discussion, Co operative learning, Problem solving

Evaluation Criteria

As per UGC guidelines on adoption of CBCS