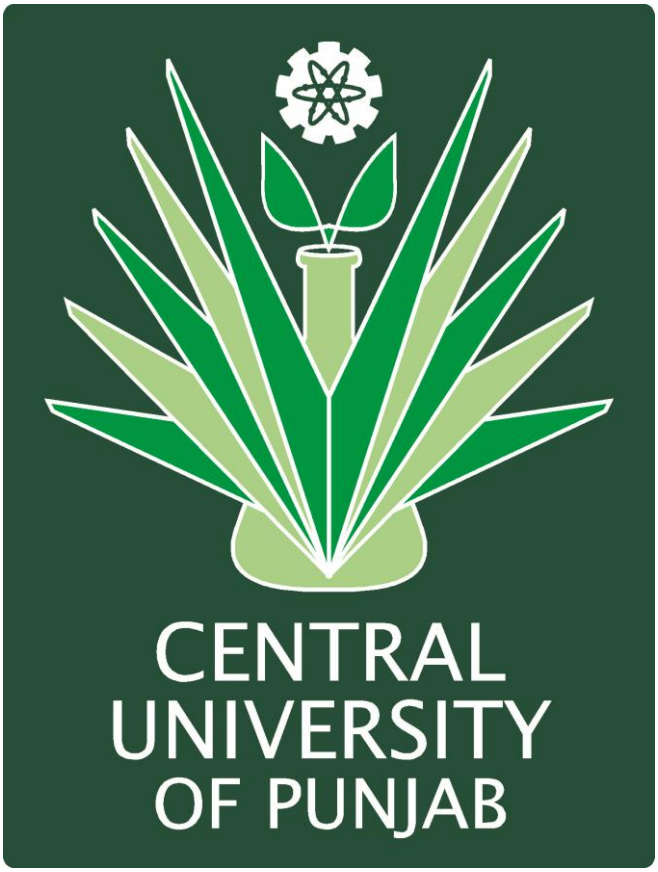
Central University of Punjab, Bathinda



M.Sc. Chemistry (Computational Chemistry)

Session 2019-2021

Department of Computational Sciences

Eligibility Criterion for MSc Chemistry (Computational Chemistry) as approved by BOS

Bachelor's degree in any branch of Chemical Sciences with 55% marks from a recognized Indian or foreign university.

Certificate

The BOS of Department of Computational Sciences certifies that the syllabus of M.Sc. Chemistry (Computational Chemistry) has been designed to ensure maximal overlap with the CSIR-UGC NET.

Programme Outcomes or Expected Skill Development among Students of MSc Chemistry (Computational Chemistry)

In line with the syllabus of MSc Chemistry (Computational Chemistry) it is expected that a student graduating after successful completion of the course shall be

1. Proficient in various aspects of Computational Chemistry.
2. Competent to carry out understanding complex information from the concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology and carry out the unsupervised research.
3. Shall have scientific temperament.

Multiple courses shall be opted by students from other (allied) departments, however, concerned teacher shall have to use examples from relevant discipline so as to gravitate the students more towards Computational Chemistry.

Therefore graduated students of MSc Chemistry (Computational Chemistry) would be a valuable asset for nation by virtue of his/her scientific abilities. The student can expect gainful employment in academic/research/industry by undertaking this programme. A special effort has been made to enable the student clear national level tests, especially, CSIR-NET.

SEMESTER I

S. No.	Paper Code	Course Title	Course Type	Hours			
				L	T	P	Cr
1	LBI.508	Basics of Biochemistry	CF	2	-	-	2
2	CCC.507	Mathematics for Chemists	CF	4	-	-	4
3	CCC.508	Scientific Programming	CF	4	-	-	4
4	LBI.515	Programming 1	CF	2	-	-	2
5	CCC.515	Scientific Programming (Practical)	CC	-	-	6	3
6	LBI.516	Programming-I Lab	CC	-	-	6	3
7	XXX	Interdisciplinary Elective	IDE	2	-	-	2
Choose any one of these courses:							
8	CCC.509	Inorganic Chemistry-I	DSE	3	-	-	3
9	CCC.510	Organic Chemistry-I	DSE	3	-	-	3
10	CCC.513	Statistics for Chemical and Biochemical Applications	DSE	3	-	-	3
11	CCC.514	Physical Organic Chemistry	DSE	3	-	-	3
12	CCC.517	Physical Chemistry-I	DSE	3	-	-	3
Interdisciplinary course offered for other centres:							
12	CCC.516	Chemistry without test tube	IDE	2	-	-	2
	Total			**23 Credits**			

SEMESTER II

S. No.	Course Code	Course Title	Course Type	Hours			
				L	T	P	Cr
1	CCC.526	Quantum Chemistry - I	CC	4	-	-	4
2	CCC.524	Statistical Mechanics - I	CC	4	-	-	4
3	CCC.523	Physical Chemistry-II	CC	3	-	-	3
4	CCC.525	Computational Methods	CC	4	-	-	4
5	CCC.528	Computational Methods Lab (Practical)	CC	-	-	6	3
6	CCC.542	Credit Seminar 1	SBE	-	-	2	1
7	XXX	Interdisciplinary Elective	IDE	2	-	-	2
Choose any one of these courses:							
9	CCC.521	Inorganic Chemistry-II	DSE	3	-	-	3
10	CCC.522	Organic Chemistry-II	DSE	3	-	-	3
11	CCC.529	Density Functional Theory	DSE	3	-	-	3
12	CCC.530	Introduction to Quantum Dynamics	DSE	3	-	-	3
	Total		**24 Credits**				

Mode of Transaction

Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning.

Evaluation Criteria

As per UGC guidelines on adoption of CBCS.

SEMESTER III

S. No.	Paper Code	Course Title	Course Type	Hours			
				L	T	P	Cr
1	CCC.556	Electronic Structure Theory	CC	4	-	-	4
2	CCC.554	Fundamentals of Molecular Simulations	CC	4	-	-	4
3	CCC.555	Molecular Simulations Lab (Practical)	CC	-	-	6	3
	CCC.557	Molecular Spectroscopy	CC	4	-	-	4
4	CCC.558	Electronic Structure Theory Lab-I (Practical)	CC	-	-	4	2
Any one of the two (in 5)							
5	CCC.599	M.Sc. Project	SBE	-	-	-	6
	CCC.600	Dissertation-I	SBE	-	-	-	6
6	XXX	Value Added Course	EF	1			1
	Total			**24 credits**			

SEMESTER IV

S. No.	Paper Code	Course Title	Course Type	Hours			
				L	**T**	**P**	**Cr**
1	CCC.575	Advanced Molecular Simulation Lab (Practical)	CC	-	-	8	4
2	CCC.572	Electronic Structure Theory Lab-II (Practical)	CC	-	-	8	4
2	CCC.574	Advanced Statistical Mechanicsand Molecular Reaction Dynamics	CC	4	-	-	4
Any one of the two (in 3)							
3	CCC.599	M. Sc. Project	SBE	-	-	-	6
	CCC.600	Dissertation Work - II	SBE	-	-	-	6
4.	XXX	Value Added Course	EF	1			1
5	CCC.544	Credit Seminar-II	SBE	-	-	1	1
Total				**20 Credits**			

Mode of Transaction

Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning.

Evaluation Criteria

As per UGC guidelines on adoption of CBCS.

a: Continuous Assessment: Subjective by enlarge

b: Mid-Term Test-1: Based on Objective Type & Subjective Type Test

c: Mid-Term Test-2: Based on Objective Type & Subjective Type Test

d: Surprise Test - 1: Based on Objective Type Test

e: Surprise Test – 2: Based on Objective Type Test

f: End-Term Exam (Final): Based on Objective Type Tests

g: Total Marks

CC: 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

SEMESTER- I

Course Title: Basics of Biochemistry
Paper Code: LBI.508
Total Hours: 30

L	T	P	Cr
2	0	0	2

Course Objective: By the end of the course, students will have gained a fundamental understanding of Biochemistry. Biochemistry is a fundamental subject, necessary for gaining insights into the application possibilities of Bioinformatics ranging from sub-cellular to large systems.

Learning Outcomes: The outcomes of the subject is to ensure that a student comprehends the following:

a) The structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles.
b) The energy metabolism by cellular components in cells and the process of mitotic cell division.
c) Influences of changes or losses in cell function; including the responses to environmental or physiological changes, or alterations of cell function brought about by mutation.

Unit 1 **8 Hours**

Principles of biophysical chemistry Thermodynamics, Colligative properties, Stabilizing interactions: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interaction, etc.

Unit 2 **6 Hours**

Composition, structure, function and metabolism of Carbohydrates, Lipids.

Unit 3 **6 Hours**

Composition, structure, function and metabolism of Amino Acids and Nucleotides.

Unit 4 **8 Hours**

Enzymology: Classification, Principles of catalysis, Mechanism of enzyme catalysis, Enzyme kinetics, Enzyme regulation, Isozymes.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings:

1. Berg, J.M., Tymoczko, J.L. and Stryer, L. (2010). *Biochemistry.* W.H. Freeman & Company. USA.
2. Brown, T.A. (2006). *Gene Cloning and DNA analysis: In Introduction.* Blackwell Publishing Professional. USA.
3. Haynie, D.T. (2007). *Biological thermodynamics.* Cambridge University. UK.
4. Mathews, C.K., Van Holde, K.E. and Ahern, K.G. (2000). *Biochemistry.* Oxford University Press Inc. New York.
5. Nelson, D. and Cox, M.M. (2013). *Lehninger Principles of Biochemistry.* BI publications Pvt. Ltd. Chennai, India.
6. Ochiai, E. (2008). *Bioinorganic chemistry: A survey.* Academic Press. Elsevier, India.
7. Randall, D. J., Burggren, W. and French, K. (2001). *Eckert animal physiology.* W.H. Freeman & Company. USA.
8. Raven, P.H., Johnson, G.B. and Mason, K.A. (2007). *Biology.* Mcgraw-Hill. USA.
9. Shukla AN (2009). *Elements of enzymology.* Discovery Publishing. New Delhi, India.
10. Voet, D. and Voet, J.G. (2014). *Principles of biochemistry.* CBS Publishers & Distributors. New Delhi, India.

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

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to:

1. identify and describe the basic mathematical techniques that are commonly used by chemist.
2. develop skills in vectors, matrices, differential calculus, integral calculus and probability.
3. apply the principles to a number of simple problems that have analytical solutions.
4. design different methods to problems related to chemistry.

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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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: Scientific Programming
Paper Code: CCC.508
Total Hours: 60

L	T	P	Cr
4	0	0	4

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Learning Outcomes: At the end of the course, the students will be able to:

- identify and describe the basic art of scientific programming related to Fortran 95/2003.
- concepts related to variables, I/O, arrays, procedures, modules, pointers and parallel programming.
- develop skills to write programs related to standard problems and as well as to chemistry.

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: Programming I
Paper Code: LBI.515
Total Hours: 30

L	T	P	Cr
2	0	0	2

Course Objective

By the end of the course, students will have gained a fundamental understanding of programming in Python by creating a variety of scripts and applications for the Web and for systems development. Python is a versatile programming language, suitable for projects ranging from small scripts to large systems. This course emphasizes best practices such as version control, unit testing and recommended styles and idioms. Students will explore the large standard library of Python 3, which supports many common programming tasks.

Learning Outcomes:

Upon successfully completing this course, students will be able to "do something useful with Python".

- Identify/characterize/define a problem
- Design a program to solve the problem
- Create pseudo executable code
- Read most of the basic Python code

Unit1 **8 Hours**

Introduction, gitHub, Functions, Booleans and Modules, Sequences, Iteration and String Formatting, Dictionaries, Sets, and Files

Unit 2 **8 Hours**

Exceptions, Testing, Comprehensions, Advanced Argument Passing, Lambda -- functions as objects

Unit 3 **7 Hours**

Object Oriented Programming, More OO -- Properties, Special methods

Unit 4 **7 Hours**

Iterators, Iterables, and Generators, Decorators, Context Managers, Regular Expressions, and Wrap Up

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Reading and resources

1. **Core Python Programming** (http://corepython.com/): Only available as a dead trees version, but if you like to have book to hold in your hands anyway, this is the best textbook style introduction out there. It starts from the beginning, but gets into the full language. Published in 2009, but still in print, with updated appendixes available for new language features. In the third edition, "the contents have been cleaned up and retrofitted w/Python 3 examples paired w/their 2.x friends."

2. Dive Into Python 3 (http://www.diveinto.org/python3/): This book offers an introduction to Python aimed at the student who has experience programming in another language.
3. Python for You and Me (http://pymbook.readthedocs.org/en/latest/): Simple and clear. This is a great book for absolute newcomers, or to keep as a quick reference as you get used to the language. The latest version is Python 3.
4. Think Python (http://greenteapress.com/thinkpython/): Methodical and complete. This book offers a very "computer science"-style introduction to Python. It is really an intro to Python in the service of Computer Science, though, so while helpful for the absolute newcomer, it isn't quite as "pythonic" as it might be.
5. Python 101 (http://www.blog.pythonlibrary.org/2014/06/03/python-101-book-published-today/) Available as a reasonably priced ebook. This is a new one from a popular Blogger about Python. Lots of practical examples. Also avaiable as a Kindle book: http://www.amazon.com/Python-101-Michael-Driscoll-ebook/dp/B00KQTFHNK
6. Problem Solving with Algorithms and Data Structures (http://interactivepython.org/runestone/static/pythonds/index.html(Links to an external site.)Links to an external site.)
7. Python Course (http://www.python-course.eu/python3_course.php(Links to an external site.)Links to an external site.)

References for getting better, once you know the basics

1. **Python Essential Reference** (http://www.dabeaz.com/per.html): The definitive reference for both Python and much of the standard library.
2. **Hitchhikers Guide to Python** (http://docs.python-guide.org/en/latest): Under active development, and still somewhat incomplete, but there is good stuff.
3. **Writing Idiomatic Python** (https://www.jeffknupp.com/writing-idiomatic-python-ebook): Focused on not just getting the code to work, but how to write it in a really "Pythonic" way.
4. **Fluent Python** (http://shop.oreilly.com/product/0636920032519.do): All python3, and focused on getting the advanced details right. Good place to go once you've got the basics down.
5. **Python 3 Object Oriented Programming** (https://www.packtpub.com/application-development/python-3-object-oriented-programming (Links to an external site.)Links to an external site.): Nice book specifically about Object Oriented programming stucture, and how to do it in Python. From local Author and founder of the Puget Sound Programming Python (PuPPy) meetup group, Dusty Phillips.

Course Title: Scientific Programming Lab (Practical)
Paper Code: CCC.515
Total Hours: 90

L	T	P	Cr
-	-	6	3

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. The students after completion of this course will be able to:

- Identify/characterize/define a computational problem
- Design a fortran program to solve the problem
- Create pseudo executable code
- Read most of the basic fortran code

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

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

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: Physical Chemistry I
Paper Code: CCC.517
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course, the students will be able to:

- Undestand the thermodynamics, phase transition, fugacity, solid and liquid transitions.
- identify and describe thermodynamical properties of a system.
- apply thermodynamical properties for various systems.
- use the knowledge of phase equilibria for various systems.
- understand how the computational techniques can be applied to study problems in advanced physical chemistry.

Unit 1 **9 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, CO_2 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 **13 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 **13 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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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: Inorganic Chemistry I
Paper Code: CCC.509
Total Hours: 45

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 1 **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.

Unit 2 **10 Hours**

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.

Unit 3 **12 Hours**

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 **13 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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 2ndedition, 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, SpringerverlagNew York Inc., 1977.
6. Miessler,G. L.andTarr, D. A. Inorganic Chemistry,4thedition, 2011, Pearson Education.
7. Figgis,B.N. Introduction to Ligand Field, 1966Wiley Eastern.
8. Drago,R.S. Physical Method in Chemistry, 1965, W.B. Saunders Company.
9. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5thedition, 2010, Oxford University Press.
10. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
11. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2ndedition, 1993, Affiliated East West Press.
12. Drago, R. S. Physical Methods for Chemists, 2ndedition, 1992, Saunders College Publishing.

Course Title: Organic Chemistry I
Paper Code: CCC.510
Total Hours: 45

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 S_N2, S_N1, mixed S_N2 and S_N1 and SET mechanism, the S_Ni 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 betweenS_N2 and S_N1 mechanisms.

Aromatic nucleophilic substitution: The S_NAr, 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, $LiAlH_4$, $NaBH_4$, 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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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, x^2 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.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

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

Learning outcomes: 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.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

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

Learning Outcomes: At the end of the course, the students will be able to:

- learn various theory related to complex chemical problems
- gain the knowledge about electronic structure, Pauli principle, and various theory related to polyatomic molecules
- understand the fundamental insights of molecular shape
- learn the mechanism of different organic reactions

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: N_2, CO, O_2

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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings:

1. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon,Viva Books, 2011.
2. 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
Paper Code: CCC.526
Total Lecture: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to:

- identify and describe the basic concepts of quantum mechanics.
- the connection of quantum mechanical operators to observables.
- identify the charecteristics of quantum mechanics in chemistry.
- apply the principles to a number of simple problems that have analytical solutions.
- analyze basic ideas on solving problems related to atomic and molecular structure, which will, in turn, prepare them to take the next advanced level course of Elctronic Structure Theory.

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 on 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 S**tructure:** 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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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
Paper Code: CCC.524
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to:

- apply the classical laws of thermodynamics and their application, mathematical review of classical mechanics
- learn the postulates of statistical mechanics, Liouville's Theorem, and statistical interpretation of thermodynamics
- identify the microcanonical, canonical, grant canonical and isobaric-isothermal ensembles, partition function, elementary probability theory, distributions and fluctuations
- learn the methods of statistical mechanics and their use to develop the statistics for Bose-Einstein, Fermi-Dirac and photon gases

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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings:

1. Kerson Haung, Statistical Mechanics, Wiley, 2nd Ed. (2008).
2. R. K. Pathria and P. D. Beale, Statistical mechanics, Elsevier, 3rd Ed (2011).
3. D. A. Mcquarrie, Statistical Mechanics, University Science Books (2011).
4. D. Chandler, Introduction to Statistical Mechanics, Oxford University Press (1987).

Course Title: Physical Chemistry II
Paper Code: CCC.523
Total Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course, the students will be able to:

- apply thermodynamical properties for various systems.
- interpret various electrochemical phenomena.
- identify and describe differential rate laws, integrated rate laws, temperature dependence of reaction
- rates, and reaction mechanisms and parallel and consecutive reactions
- knowledge about catalysts and catalyzed reactions.
- gain depth knowledge in this fundamental branch of chemistry.
- understand how the computational techniques can be applied to study problems in advanced physical chemistry.

Unit 1 **10 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 **10 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 **12 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 **13 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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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: Computational Methods
Paper Code: CCC.525
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to solve:

- the large scale systems of linear, non-linear and simultaneous equations
- the matrix and determinants, interpolations, polynomial and spline interpolation
- the numerical differentiation and integration
- complex curve fitting methods, explicit schemes to solve differential equations
- the 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 **15 Hours**

Linear and Non –Linear equations:
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 **16 Hours**

Interpolations:
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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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: Computational Methods lab
Paper Code: CCC.528
Total Hours: 90

L	T	P	Cr
0	0	6	3

Learning Outcomes: At the end of the course, the students will be able to:

- learn computer code for the large scale systems of transcendental and polynomial equations
- understand numerical strategies to write a computer code for the solution of matrix and determinants, interpolations, polynomial and spline interpolation
- learn the computer code for numerical differentiation and integration, differential equations, complex curve fitting, and simple optimisation

After, completion of this course will help the students to apply numerical methods to obtain approximate solutions of complex mathematical problems.

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.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

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. E. Balaguruswamy, Numerical Methods, Tata McGraw Hill (2017).
4. V. Rajaraman, Computer oriented numerical methods, PHI Learning Pvt. Ltd., 4th Ed. (2018).

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

L	T	P	Cr
3	0	0	3

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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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

Learning Outcomes: At the end of the course, the students will be able to:

- learn systematic theoretical validations of the separation of electronic and nuclear motions
- gain the knowledge about the basic aspects of time dependent quantum wavepacket dynamics
- understand various numerical methods for solving the TDSE

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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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.

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

L	T	P	Cr
0	0	2	1

Learning objective: 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 Hours: 45

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course, the students will be able to:

- learn the advanced topics in inorganic chemistry, eg symmetry operation and group theory, metal complexes, inorganic rings and cages
- 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,

Unit 2 **12 Hours**

Group theory

Determination of reducible and irreducible representations, character tables, construction of character tables for C_2v, C_3v, 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.

Unit 4 **16 Hours**

Inorganic chains, rings and cages

a) **Chains:** Catenation, heterocatenation, isopolyanions and heteropolyanions.
b) **Rings:** Borazines, phosphazenes, other heterocyclic inorganic ring systems, homocyclic
c) inorganic systems.
d) **Cages:** Cage compounds having phosphours, oxygen, nitrogen and sulphur: boron cage
e) compounds, boranes, carboranes and metallocenecarboranes.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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.
6. Carlin, R. L. and Van Duyneveldt, A.J. Magnetic Properties of Transition Metal Compounds, Inorganic Chemistry Concepts 2, Springerverlag New York Inc., 1977.
7. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5th edition, 2010, Oxford University Press.
8. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
9. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 2nd edition, 1993, Affiliated East West Press.
10. Drago, Russell S. Physical Methods for Chemists, 2nd edition, 1992, Saunders College Publishing

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

L	T	P	Cr
3	0	0	3

Learning Outcomes: At the end of the course, the students will be able to:

- learn the advanced topics in organic chemistry eg. stereochemistry, photochemistry, pericyclic and cycloaddition reaction, sigmatropic rearrangements.
- gain the knowledge of different computational techniques and its application 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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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

SEMESTER III

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

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to:

- identify and define basic terms and concepts which are needed for this specialized corse.
- describe the HF SCF method.
- choose the basis sets.
- compare post-HF methods.
- identify and define the concept of DFT.
- identify how to apply quantum chemistry to study hemical and biochemical problems.

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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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
Paper Code: CCC.554
Total Lecture: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to:

- learn the modelling of small to large molecular environments
- understand various force field for biomoleculra simulation in details
- learn different methods for simulating large systems
- gain the knowledge about different molecular simulation techniques
- understand 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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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
Total Lecture: 90

L	T	P	Cr
0	0	6	3

Learning Outcomes: At the end of the course, the students will be able to:

- learn the basics of Linux environment
- use the remote computing as a tool for high performance computation
- use different energy minimization techniques
- create molecular model from scratch, and high definition images using various graphics tools
- gain the practical in-hand experience of various modeling and classical simulation tools
- learn the use of different insilico techniques for biomolecular 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

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

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: Molecular Spectroscopy
Paper Code: CCC.557
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to:

- gain the knowledge about various spectroscopic techniques, such as, electronic, microwave, vibrational, raman, nuclear magnetic resonance, and laser spectroscopy
- understand, how spectroscopic transitions come into picture in molecular quantum mechanics
- learn various spectroscopic selection rules and their applications

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.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

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: Electronic Structure Theory Lab-I (Practical)
Paper Code: CCC.558
Total Hours: 60

L	T	P	Cr
0	0	4	2

Course Learning Outcomes: This course will provide practical experience to the students through use of important Computational Chemistry softwares related to electronic structure theory.

Following experiments will be carried out in the lab.

1. Introduction to electronic structre calculations.
2. Basis set dependency.
3. HF and DFT methods related calculations.
4. Carrying of conformational analysis of small molecules.
5. MO and charge distribution calculations.
6. Vibrational spectra calculations.
7. 2D potential energy suface generation.
8. Transition state calculations.
9. Absorption spectra study.
10. Calculations using solvent.
11. Thermochemistry study.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Suggested Readings:

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
4. http://ambermd.org/tutorials/

Course Title: M.Sc. Dissertation I
Paper Code: CCC.600
Invested Hours: 180

L	T	P	Cr
0	0	12	6

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. VC nominee
c. Supervisor (and Co-supervisor if applicable)

*of as recommended by School Board.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

SEMESTER IV

Course Title: Advanced Statistical Mechanics and Molecular Reaction Dynamics
Paper Code: CCC.574
Total Hours: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: At the end of the course, the students will be able to:

- identify and define basic terms and concepts of Phase transitions
- describe the Non-equilibrium dynamics
- learn the behavior of systems not far from equilibrium
- create potential energy surfaces for different small molecules
- explain the energetics of transition statesof reactions

Unit I **18 Hours**

Review of Statistical Mechanical concepts, Phases & Phase Transitions: The Ising Model : Stability of Thermodynamics Phases, First-order Phase transitions, Interfaces, The Ising Model, Lattice Gas, Broken Symmetry, Mean Field Theory.

A brief introduction to Liquid Theory: Averages, Distribution Functions, Reversible Work Theorem, Radial distribution function, Molecular liquids

Atomic and continuum models of liquids: The Lennard-Jones Fluid, Molecular dynamics simulation, Correlation functions and measurements, elements of linear response theory, Linear models (a) Langevin equations (diffusion, friction and memory). (b) Gaussian fields (Debye-Huckel and beyond), The hard sphere model, WCA theory, Chemical equilibrium and relaxation.

Unit II **18 Hours**

Non-equilibrium systems: Fluctuation-Dissipation Theorem, Onsager's Regression Hypothesis

Brownian Motion, Friction and the Langevin Equation, Transport, Time Correlation Functions.

Special topics: Free energy perturbation, The Jarzynski Equality, Electron transfer--quantum rare events--golden rule--Marcus theory, Path integrals, Tunneling—instantons, Ising model / Quantum correspondence, Monte Carlo and Biased Monte Carlo methods.

Unit III **18 Hours**

Potential Energy Surfaces: Long-range Potentials, Empirical Intermolecular Potentials, Molecular Bonding Potentials, Internal Coordinates and Normal Modes of Vibration, Ab Initio Calculation of Potential Energy Surfaces, Analytic Potential Energy Functions, Details of the Reaction Path.Dynamics of Bimolecular Collisions: Simple Collision Models, Two-Body Classical Scattering, Complex Scattering Process.

Unit IV **18 Hours**

Transition State Theory: Basic Postulates and Derivation of Transition State Theory, Dynamical Derivation of Transition State Theory, Quantum Mechanical Effects in Transition State Theory, Thermodynamic Formulation of Transition State Theory, Applications of Transition State Theory.Unimolecular Reaction Dynamics: The Lindmann-Hinshelwood Mechanism, Statistical Energy-dependent Rate Constant, RRKM Theory, Applications of RRKM Theory to Thermal Activation.

Transactional Modes: Lecture; Tutorial; Problem solving; Self-learning.

Suggested Readings:

1. Kerson Haung, Statistical Mechanics, Wiley, 2nd Ed. (2008).
2. R. K. Pathria and P. D. Beale, Statistical mechanics, Elsevier, 3rd Ed (2011).
3. B. K. Agarwal and M. Eisner, Statistical Mechanics, Wiley Eastern, New Delhi (1998).

4. D. A. Mcquarrie, Statistical Mechanics, University Science Books (2011).
5. D. Chandler, Introduction to Statistical Mechanics, Oxford University Press (1987).
6. B. Widom, Statistical Mechanics- A concise Introduction for Chemists, Cambridge University Press (2002).
7. Terrell L. Hill, Statistical mechanics: principles and selected applications, Courier DoverPublications (1987).
8. J. I. Steinfeld, J. S. Francisco, and W. L. Hase, Chemical Kinetics and Dynamics, Prentice Hall (1998).
9. R. D. Levine, Molecular Reaction Dynamics, Cambridge University Press (2009).
10. N. E. Henriksen F. Y. Hansen, Theories of Molecular Reaction Dynamics: The Microscopic Foundation of Chemical Kinetics, Oxford University Press, USA (2012).
11. M. Brouard, Reaction Dynamics, Oxford Chemistry Primers (1998).
12. P. L. Houston, Chemical Kinetics and Reaction Dynamics, Dover Publications (2012).
13. S. K. Upadhyay, Chemical Kinetics and Reaction Dynamics, Springer (2006).
14. K. J. Laidler, Chemical Kinetics, Pearson (2008).
15. H. Zewail, Femtochemistry-Ultrafast Dynamics of the Chemical Bond, World Scientific, New Jersey (1994).

Course Title: Advanced Molecular Simulation Lab
Paper Code: CCC.575
Total Hours: 90

L	T	P	Cr
0	0	8	4

Learning Outcomes: At the end of the course, the students will be able to:

- learn various tools for protein structure prediction
- learn the homology and comparative modeling techniques
- understand the effect of sequence on the molecular model building
- learn the structure based drug designing
- gain the knowledge about various advanced molecular modeling techniques

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

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Suggested Readings:

1. Andrew R.Leach Molecular Modelling Principles and applications, (2009) II ed . Pearson Education.
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 - II (Practical)
Paper Code: CCC.572
Total Hours: 120

L	T	P	Cr
0	0	8	4

Learning Outcomes: This course will provide practical experience to the students through use of important Computational Chemistry softwares related to electronic structure theory.

Following experiments will be carried out in the lab.

1. Post-HF based calculations
2. Studying potential energy surface.
3. Carrying of conformational analysis of large systems.
4. Model chemistry.
5. Study of NMR spectra
6. Fluorescence and photoelectron spectra.
7. Modeling chemical reactions using classical dynamics.
8. Elctronic circular dichroism study.
9. Boltzmann averaging.
10. Pseudopotential generation and testing of Si atom.
11. QM/MM study.
12. Inclusion of Relativistic effects.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.

Suggested Readings:

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
4. http://ambermd.org/tutorials/

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. Dissertation II
Paper Code: CCC.600
Total Hours: 240

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:

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. VC nominee
c. Supervisor (and Co-supervisor if applicable)

*of as recommended by School Board.

Transactional Modes: Laboratory based practicals; Problem solving; Self-learning.