Central University of Punjab, Bathinda

M.Sc. Chemistry (Computational Chemistry)

Session: 2020-2022

Department of Computational Sciences

School of Basic and Applied Sciences

Programme Outcomes (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 able to:

1. learn a deep knowledge in various areas of Theoretical and Computational Chemistry, basic knowledge in Mathematics, and knowledge in applied fields like Computer Science.
2. demonstrate the knowledge, general competence, and analytical skills on an advanced level, needed in industry, consultancy, education, research, or public administration.
3. extract complex information from the concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology, and successfully carry out research assignment and projects, both independently and in collaboration with others.

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.

Course Structure of the Programme

SEMESTER I							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	CCC.524	Statistical Mechanics	CC	4	0	0	4
2	LBI.508	Basics of Biochemistry	CF	2	0	0	2
3	PCP.506	Mathematics for Computational Sciences	CF	4	0	0	4
Choose any one of these courses							
4	CCC.509	Inorganic Chemistry-I	DE	4	0	0	4
5	CCC.510	Organic Chemistry-I	DE	4	0	0	4
6	CCC.513	Statistics for Chemical and Biochemical Applications	DE	4	0	0	4
7	CCC.514	Physical Organic Chemistry	DE	4	0	0	4
8	CCC.517	Physical Chemistry	DE	4	0	0	4
Choose any one (theory and related lab) of these courses							
4	CCC.508	Scientific Programming	DE	4	0	0	4
5	CCC.515	Scientific Programming (Practical)	SBE	0	0	8	4
6	LBI.515	Programming 1	DE	4	0	0	4
7	LBI.516	Programming-I Lab	SBE	0	0	8	4
8	XXX	Interdisciplinary Course	IDC	2	0	0	2
Interdisciplinary course offered for other departments							
	CCC.516	Chemistry without test tube	IDC	2	0	0	2
Total				**20**	**0**	**8**	**24**

SEMESTER II							
S. No.	**Course Code**	**Course Title**	**Course Type**	**Hours**			
				L	**T**	**P**	**Cr**
1	PCP.525	Solid State Physics	CC	4	0	0	4
2	PCP.526	Computational Solid State Physics Laboratory	SBC	0	0	6	3
3	CCC.525	Computational Methods	CC	4	0	0	4
4	CCC.528	Computational Methods Lab (Practical)	SBC	0	0	8	4
5	PCP.527	Quantum Mechanics	CC	4	0	0	4
6	CCC.542	Seminar	SBE	0	0	0	1
7	XXX	Interdisciplinary Course	IDC	2	0	0	2
Interdisciplinary course offered for other departments							
	CCC.516	Chemistry without test tube	IDC	2	0	0	2
Choose any one of these courses/MOOC							
8	CCC.521	Inorganic Chemistry-II	DE	4	0	0	4

9	CCC.522	Organic Chemistry-II	DE	4	0	0	4
10	CCC.529	Density Functional Theory	DE	4	0	0	4
11	CCC.530	Introduction to Quantum Dynamics	DE	4	0	0	4
Total				**18**	**0**	**14**	**26**

SEMESTER III							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	T	P	Cr
1	CCC.556	Electronic Structure Theory	CC	4	0	0	4
2	CCC.554	Fundamentals of Molecular Simulations	CC	4	0	0	4
3	CCC.555	Molecular Simulations Lab (Practical)	SBC	0	0	8	4
4	PCP.557	Atomic and Molecular Spectroscopy	CC	4	0	0	4
5	CCC.599	M.Sc. Project - I	SBE	0	0	0	6
6	CCC.559	Introduction to Molecular Docking	VAC	1	0	0	1
Total				**13**	**0**	**8**	**23**

SEMESTER IV							
S. No.	**Paper Code**	**Course Title**	**Course Type**	**Hours**			
				L	**T**	**P**	**Cr**
1	CCC.573	Electronic Structure Theory Lab (Practical)	SBC	0	0	8	4
2	CCC.571	Enrich Chemistry Course - I	DEC	2	0	0	2
3	CCC.572	Enrich Chemistry Course - II	DEC	2	0	0	2
Choose any one (theory and related lab) of these courses							
4	CCC.575	Advanced Molecular Simulation Lab	DE	0	0	8	4
5	CCC.574	Advanced Statistical Mechanics and Molecular Reaction Dynamics	DE	4	0	0	4
6	CCC.576	Biomolecular Structure Modelling	DE	4	0	0	4
7	CCC.577	Practicals in Biomolecular Structure Modeling	DE	0	0	8	4
8	LBI.574	Bioinformatics for Transcriptomics and Metabolomics	VAC	1	0	0	1
9	CCC.599	M. Sc. Project - II	SBE	0	0	0	6
Total				**9**	**0**	**16**	**23**

Grand Total	96 Credits

Mode of Transaction: Lecture, Laboratory based Practical, Seminar, Group discussion, Team teaching, Self-learning.

Evaluation Criteria for Theory Courses

A. Continuous Assessment: [25 Marks]
   i. Surprise Test (minimum three) - Based on Objective Type Tests (10 Marks)
   ii. Term paper (10 Marks)
   iii. Assignment(s) (5 Marks)

B. Mid Semester Test-1: Based on Subjective Type Test [25 Marks]
C. End Semester Test-2: Based on Subjective Type Test [25 Marks]
D. End-Term Exam: Based on Objective Type Tests [25 Marks]

*Every student has to take up 2 ID courses of 2 credits each (Total 04 credits) from other disciplines in any two semesters of the program.

CC: Core Course, VAC: Value Added Course, EP: Elective Project, SEC: Skill Enhancement Course, IDE: Interdisciplinary Elective, DE: Discipline Elective, CF: Compulsory Foundation, SBC: Skill Based Core; SBE: Skill Based Elective, VAC: Value Added Courses

L	T	P	Cr
4	0	0	4

SEMESTER- I

Course Title: Statistical Mechanics
Paper Code: CCC.524
Total Hours: 60

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.

Course Content

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

Course Title: Basics of Biochemistry

L	T	P	Cr
2	0	0	2

Paper Code: LBI.508

Total Hours: 30

Learning Outcomes: The outcomes of the subject is to ensure that the learner will be able to 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.

Course Content

Unit 1 **10 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 Computational Sciences
Paper Code: PCP.506
Total Lectures: 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 mathematical techniques that are commonly used by chemist.
- develop skills in vectors, matrices, differential calculus, integral calculus and probability.
- apply the principles to a number of simple problems that have analytical solutions.
- design different methods to problems related to chemistry.

Course Content

Unit I **15 Hours**

Matrices & Vector Calculus: matrix algebra, Caley-Hamilton theorem, Eigen values and Eigen vectors, curvilinear coordinates. (Vector calculus: properties of Gradient, divergence and Curl, spherical and cylindrical coordinates)

Differential calculus: 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.

Unit II: **15 Hours**

Integral calculus: 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

Fourier Transforms: Fourier series, Dirichlet condition, General properties of Fourier series, Fourier transforms, their properties and applications,

Unit III: **14 Hours**

Delta, Gamma, and Beta Functions: Dirac delta function, Properties of delta function, Gamma function, Properties of Gamma and Beta functions.

Special Functions: Legendre, Bessel, Hermite and Laguerre functions, recurrence relations, Orthogonality and special properties. Associated Legendre functions: recurrence relations, Parity and orthogonality, functions, Green's function,

Unit IV: **16 Hours**

Differential Equations Solutions of Hermite, Legendre, Bessel and Laugerre Differential equations, basics properties of their polynomials, and associated Legendre polynomials, Partial differential equations (Laplace, wave and heat equation in two and three dimensions), Boundary value problems and Euler equation.

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

Suggested Readings

1. E. Kreyszig, *Advanced Engineering Mathematics* (Wiley India Pvt. Ltd., New Delhi, India) 2011.
2. L. A. Pipes, *Applied Mathematics for Engineers and Physicist* (McGraw-Hill, Noida, India) 1985.
3. D. G. Zill, *Advanced Engineering Mathematics* (Jones & Barlett Learning, Massachusetts, USA) 2012.
4. P. K. Chattopadhyay, *Mathematical Physics* (New Age International (P) Ltd., New Delhi) 2000
5. The chemistry Mathematics Book, E.Steiner, Oxford University Press (2008).
6. Mathematical for Physical Chemistry : F. Daniels, Mc. Graw Hill (1959).

7. Chemical Mathematics D.M. Hirst, Longman (1979).
8. Basic Mathematics for Chemists, Tebbutt, Wiley (1994).
9. G. Arfken, H. Weber and F. Harris, *Mathematical Methods for Physicists* (Elsevier Academic Press, Massachusetts, USA) 2012.

Course Title: Inorganic Chemistry I
Paper Code: CCC.509
Total Lectures: 60

L	T	P	Cr
4	0	0	4

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.

Course Content

Unit 1 **14 Hours**

Metal-Ligand Equilibria in Solution

tepwise 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 **14 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 **16 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 **16 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, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2005 (reprinted),Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 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, 2010, Oxford University Press.
10. Earnshaw, A. Introduction to Magnetochemistry, 1968, Academic Press.
11. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 1993, Affiliated East West Press.
12. Drago, R. S. Physical Methods for Chemists, 1992, Saunders College Publishing.

L	T	P	Cr
4	0	0	4

Course Title: Organic Chemistry I
Paper Code: CCC.510
Total Hours: 60

Learning Outcomes: The outcomes of this course is that students will be learned the reaction mechanism and its intermediates, aromaticity, different

sets of aliphatic nucleophilic reaction, aromatic nucleophilic 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.

Course Content

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 **16 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 **14 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, 2012, Oxford University Press.
2. Finar, I.L. Organic Chemistry Volume 1, 2012, Pearson Education UK.
3. McMurry J. Organic Chemistry, 2011 Asian Book Pvt. Ltd, New Delhi
4. Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 2013, John Wiley & Sons.
5. Ahluwalia, V. K. and Parashar R. K. Organic Reaction Mechanism, 2011, Narosa Publishing House (P) Ltd., New Delhi.
6. Bansal, R. K. A text book of Organic Chemistry, 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. 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, 1998, Addison-Wesley Longman Inc., New York.
11. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 2011, Prentice-Hall of India, New Delhi.
12. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 2009, Macmillan India Ltd., New Delhi.
13. Robert, J. D. and Casereo, M.C. Basic principle of Organic Chemistry, 1977, Addison-Wesley.
14. Solomon, T.W.G, Fryhle, C.B. and Snyder, S. A.Organic Chemistry. 2013, John Wiley and Sons, Inc.
15. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 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: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: This course will introduce the basic aspects of various industry based statistical methods to students which will be used to compare different results.

Course Content

Unit I **14 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 **16 Hours**

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

Unit III **14 Hours**

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

Unit IV **16 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.

L	T	P	Cr
4	0	0	4

Course Title: Physical Organic Chemistry
Paper Code: CCC.514
Total Lecture: 60

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.

Course Content

Unit-I **14 Hours**

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

Unit-II **16 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 **14 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 **16 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*, 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, Springer, 2007.
4. Jerry March, *Advanced Organic Chemistry, Reactions, Mechanims and Structure*, John-Wiley, 1999.
5. Thomas H. Lowry, Kathleen S. Richardson, *Mechanism and Theory in Organic Chemistry*, Harper & Row, 1981.
6. S. P. Gupta, *QSAR and Molecular Modeling*, Anamaya Publishers, 2011.

L	T	P	Cr
4	0	0	4

Course Title: Physical Chemistry
Paper Code: CCC.517
Total Hours: 60

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.
- investigate how the computational techniques can be applied to study problems in advanced physical chemistry.
- 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.

Course Content

Unit 1 **14 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 2 **14 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 **16 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 4 **16 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.

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, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 2-3,5, 2011, Macmillan.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1998, Viva Books.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 1981, John Wiley and Sons.
6. Engel, T., Reid, P. and Hehre, W. Physical Chemistry, 2012, Pearson Education.
7. Rastogi, R. P. and Mishra, R. R. An Introduction to Chemical Thermodynamics, 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, 2012, Dover Publication Inc.
11. Hill, T. L. An Introduction to Statistical Thermodynamics, 1986, Dover Publications Inc.

L	T	P	Cr
4	0	0	4

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

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.
- demonstrate 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.

Course Content

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 arrays 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 parallel programming, Parallel Architecture, Open MP & MPI, Models of Parallel Computation, Parallel Program Design, Shared Memory & Message Passing, Algorithms, Merging & Sorting.

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

Suggested Readings

1. Chapman, Fortran 95/2003 for Scientists and Engineers, 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: Scientific Programming Lab (Practical)
Paper Code: CCC.515

L	T	P	Cr
0	0	8	4

Total Hours: 120

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

Course Content

Unit I **30 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 **30 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 arrays in procedures, derived data types.

Unit III **30 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 **30 Hours**

What is parallel programming, Why use parallel 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 Engineers, 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: Programming I
Paper Code: LBI.515

L	T	P	Cr
4	0	0	4

Total Lectures: 60

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

Course Content

Unit1 **15 Hours**
Introduction, gitHub, Functions, Booleans and Modules, Sequences, Iteration and String Formatting, Dictionaries, Sets, and Files

Unit 2 **15 Hours**
Exceptions, Testing, Comprehensions, Advanced Argument Passing, Lambda -- functions as objects

Unit 3 **15 Hours**
Object Oriented Programming, More OO -- Properties, Special methods

Unit 4 **15 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.)
7. Python Course (http://www.python-course.eu/python3_course.php (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 structure, 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: Practicals in Programming I
Paper Code: LBI.516

L	T	P	Cr
0	0	8	4

Total Hours: 120

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 executable code
- Read most Python code
- Write basic unit tests

Course Content

Working with Data. A detailed tour of how to represent and work with data in Python. Covers tuples, lists, dictionaries, and sets. Students will also learn how to effectively use Python's very powerful list processing primitives such as list comprehensions. Finally, this section covers critical aspects of Python's underlying object model including variables, reference counting, copying, and type checking.

Program Organization, Functions, and Modules. More information about how to organize larger programs into functions and modules. A major focus of this section is on how to design functions that are reliable and can be easily reused across files. Also covers exception handling, script writing, and some useful standard library modules.

Classes and Objects. An introduction to object-oriented programming in Python. Describes how to create new objects, overload operators, and utilize Python special methods. Also covers basic principles of object oriented programming including inheritance and composition.

Inside the Python Object System. A detailed look at how objects are implemented in Python. Major topics include object representation, attribute binding, inheritance, memory management, and special properties of classes including properties, slots, and private attributes.

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

References for getting started

- The Python Tutorial (https://docs.python.org/3/tutorial/): This is the official tutorial from the Python website. No more authoritative source is available.
- Code Academy Python Track (http://www.codecademy.com/tracks/python): Often cited as a great resource, this site offers an entertaining and engaging approach and in-browser work.
- Learn Python the Hard Way (http://learnpythonthehardway.org/book/): Solid and gradual. This course offers a great foundation for folks who have never programmed in any language before. [Python 2]

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 Content

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, Wiley-Blackwell (2006).
4. Quantum Chemistry: A Unified Approach, D. B. Cook, 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: Solid State Physics
Paper Code: PCP.525
Total Lecture: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: The course on Solid State Physics is to provide the student with a clear and logical presentation of the basic and advanced concepts and principles of the physics for solid state.
At the end of the course, the students will be able to:

- learn the various types of crystal structure, and x-ray diffraction
- methods
- interpret the lattice vibrations and band theory of solids
- gain deep knowledge on magnetic properties of solids, defects, superconductivity
  which will help them to apply these techniques in
  investigating the aspects of the matter in condensed phase.

Course Content

Unit I **18 Hours**

Crystal Structure: Bravais lattices, Crystal structures, Reciprocal lattices, Ewald sphere, X-ray diffraction, Lattice parameter determination, Atomic and crystal structure factors, Bonding of solids, kinds of liquid crystalline order, Quasi crystals.
X-ray diffraction: X-ray diffraction, Bragg law, Laue equations, atomic form factor and structure factor. Concept of reciprocal lattice and Ewald's construction. Experimental diffraction methods: Laue rotating crystal method and powder method.

Unit II **14 Hours**

Electronic properties and band theory: Electronic structure of solids-band theory, Refinement of simple band theory- k-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, p-n junctions; superconductors, Meissner effects, basic concepts of BCH theory.

Unit III **14 Hours**

Magnetic Properties: Behavior of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis.

Unit IV **14 Hours**

Defects in solids: Point defects: Schottky and Frenkel defects and their equilibrium concentrations. Line defects: dislocations, multiplication of dislocations (Frank – Read mechanism). Plane defects grain boundary and stacking faults.
Superconductivity: Meissner effect, Type-I and type-II superconductors; BCS theory, Flux quantization, Coherence, AC and DC Josephson effect, Superfluity, High TC superconductors and their applications.

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

Recommended books

1. J. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, Cambridge, U.K.) 2011.
2. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007.
3. R.J. Singh, *Solid State Physics* (Pearson, New Delhi, India) 2011.
4. A.J. Dekker, *Solid State Physics* (Macmillan, London, U.K.) 2012.
5. N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Thomson Press), 2003.
6. A.R. Verma and O.N. Srivatava, *Crystallography Applied to Solid state physics* (New Age International), 2012

Course Title: Computational Solid State Physics Laboratory
Paper Code: PCP.526
Total Hours: 90

L	T	P	Cr
0	0	6	3

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

- learn the computational methods for CSCl crystal structure determination
- carry out the geometry optimization of molecular crystals
- measure the Infrared spectra of crystals, and Raman spectra
- interpret the dispersion relation and cut-off frequency for the mono-atomic lattice which will enhance their employability in their further potential careers in academia and industry

Course Content

1. Determine the crystal structure of CsCl using Gaussian package.
2. Geometry optimization of crystals using Gaussian package.
3. Determination of Infrared spectra of crystals using Gaussian package.
4. X-ray diffraction refinement using ICSD data.
5. Obtaining the structure of NaCl crystal system using Diamond software package.
6. Determination of Raman spectra using Gaussian package.
7. To determine magneto resistance of a bismuth crystal as a function of magnetic field.

8. Determination of critical temperature of high temperature superconductor and Meissner effect for a high Tc superconductor.
9. Determination of ferromagnetic to paramagnetic phase transition temperature (TC = Curie temperature).
10. Determination of dielectric constant of solids.
11. Study of the dispersion relation and cut-off frequency for the mono-atomic lattice. Study of the dispersion relation for the di-atomic lattice – 'acoustical mode' and 'optical mode' and energy gap.
12. Study of thermal expansion pf solids.
13. Study of thermal conductivity of solids.
14. Study of specific heat of solids.

Transactional Modes: Computation work, Experimentation and Viva-voce..

Suggested Readings

- J. Ziman, *Principles of the Theory of Solids* (Cambridge University Press, New Delhi) 2011.
- J.P. Srivastava, *Elements of Solid State Physics* (PHI Learning, New Delhi, India) 2011.
- R.J. Singh, *Solid State Physics* (Pearson, New Delhi, India) 2011.
- C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2014.

L	T	P	Cr
4	0	0	4

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

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.

Course Content

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.

L	T	P	Cr
0	0	8	4

Course Title: Computational Methods lab
Paper Code: CCC.528
Total Hours: 120

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.

Course Content

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., (2018).

L	T	P	Cr
4	0	0	4

Course Title: Quantum Mechanics
Paper Code: PCP.527
Total Lecture: 60

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 characteristics 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 Electronic Structure Theory.

Course Content

Unit I **16 Hours**

Fundamental Background: Postulates of quantum mechanics, Eigen values and Eigen functions, operators, hermitian, 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, Spin angular momentum: Pauli matrices and their properties.

Unit II **14 Hours**

Approximation methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples, WKB method, time-dependent perturbation theory, radiative transitions, Einstein coefficients.

Unit III **14 Hours**

Addition of Angular Momenta: Addition of two angular momenta, Transformation between bases: Clebsch-Gordan Coefficients, Eigenvalues of J^2 and Jz, Coupling of orbital and spin angular momenta.

Unit IV **16 Hours**

Scattering Theory: Quantum Scattering theory, Scattering cross-section and scattering amplitude, Born scattering formula, Central force problem, Partial wave analysis, Phase shifts, Optical theorem, Low energy s-wave and p-wave scatterings, bound states and resonances

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

Suggested Readings

1. Quantum Chemistry, I.N. Levine, 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, John Wiley (1965).
4. Introductory Quantum Chemistry, A.K. Chandra, 4th Edition, Tata Mcgraw Hill (1994).
5. N. Zettili, *Quantum Mechanics-Concepts and Applications* (John Wiley & Sons Ltd., Sussex, U.K.) 2009.
6. E. Merzbacher, *Quantum Mechanics* (Wiley India Pvt. Ltd., New Delhi, India) 2011.
7. J. J. Sakurai, *Modern Quantum Mechanics* (Pearson Education, India) 2009.
8. D. J. Griffiths, *Introduction to Quantum Mechanics*, (Pearson Education, India) 2015.
9. G. D. Mahan, Quantum Mechanics in a Nutshell (Princeton University Press) 2009.
10. Quantum Chemistry, J. P. Lowe, and Peterson, K., Academic Press (2005).

Course Title: Seminar
Paper Code: CCC.542

L	T	P	Cr
0	0	0	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:

Continious Evaluation:

S.No.	Criteria	Marks
1.	Knowledge of Subject: In depth coverage, ability to interpret science	25
2.	Questions: Understanding of questions, ability to reply with logic	25
End Term:		
1.	(a) Presentation: Voice, Ability to command attention, (b) Handling of queries	50
	Total	**100**

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

Course Content

Unit 1 **14 Hours**

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

Unit 2 **14 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 **16 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 inorganic systems.
c) **Cages:** Cage compounds having phosphours, oxygen, nitrogen and sulphur: boron cage compounds, boranes, carboranes and metallocenecarboranes.

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

Suggested Readings

1. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 2007, John Wiley& Sons.
2. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 2006, Dorling Kindersley (India) Pvt. Ltd.
3. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd.
4. Lever, A.B.P. Inorganic Electronic Spectroscopy, 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, 1993, Affiliated East West Press.
9. Drago, Russell S. Physical Methods for Chemists, 1992, Saunders College Publishing

Course Title: Organic Chemistry II
Paper Code: CCC.522
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:

- 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.

Course Content

Unit 1 **16 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 **14 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, 1976 Wiley India Pvt. Ltd.
2. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2012, Oxford University Press.
3. Ahluwalia, V. K. and Parasar R. K. Organic Reaction Mechanism, 2011, Narosa Publishing House (P) Ltd., New Delhi.
4. Bansal, R. K. A Textbook of Organic Chemistry, 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, 2010, New Age International (P) Ltd., New Delhi.
7. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part A, 2002, Kluwer Academic Publishers.
8. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part B, 2007, Springer Science and Business Media Ltd.
9. Finar, I.L. Organic Chemistry Volume 1, 2012, Pearson Education UK.
10. Gilchrist, T.L. (1997). Heterocyclic Chemistry, 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, 2010, Blackwell Publishers, New York.
13. Kalsi, P.S. Organic Reactions and Their Mechanisms. 2010, New Age International, New Delhi.
14. Lowry, T. H. and Richardson K. S. Mechanism and Theory in Organic Chemistry, 1998, Addison-Wesley Longman Inc., New York.
15. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 2011, Prentice- Hall of India, New Delhi.
16. Mukherjee, S.M. and Singh, S.P. Reaction Mechanism in Organic Chemistry. 2009, Macmillan India Ltd., New Delhi.
17. Katritzky, A. R., Ramsden, C. A., Joule, J. A. and Zhdankin V. V. Handbook of Heterocyclic Chemistry, 2010, Elsevier UK.
18. Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 2013, John Wiley & Sons.
19. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 1997, Prentice Hall.
20. Norman, R.O.C. and Coxon, J.M. Principles of Organic Synthesis, 1998, Nelson Thornes, Blackie Academic & Professional.

Course Title: Density Functional Theory
Paper Code: CCC.529
Total Lecture: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: This is a specialization course for students of Computational Chemistry. At the end of the course, the students will be able to:

- learn basics of Density Functional Theory (DFT)
- understand most popular framework of modern DFT.
- characterize the properties of molecules and materials
  After completion of this course, it will help the students to use different functional appropriately for different problems.

Course Content

Unit-I **14 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 **15 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 **16 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 **15 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: 60

L	T	P	Cr
4	0	0	4

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

Course Content

Unit I **15 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 **15 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 **15 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 **15 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.

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 course.
- 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 chemical and biochemical problems.

Course Content

Unit I **16 Hours**

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

Unit II **14 Hours**

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

Unit III **15 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, Wiley-Blackwell (2006).
2. Molecular Quantum Mechanics, P. W. Atkins and R. S. Friedman, 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, (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 biomolecular 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.

Course Content

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 Hours: 120

L	T	P	Cr
0	0	8	4

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 carriers in academia and industry

Course Content

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) . 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: Atomic and Molecular Spectroscopy
Paper Code: PCP.557
Total Lectures: 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

Course Content

Unit I **14 Hours**

Atomic Spectra: Revision of quantum numbers, electron configuration, Hund's rule etc. origin of spectral lines, LS & JJ coupling , selection rules, Spectrum of hydrogen, helium and alkali atoms, X-ray spectra, fine spectra, hyperfine structure, Width of spectrum lines.

Unit II **16 Hours**

Molecular Spectra: Molecular potential, Separation of electronic and nuclear wave functions, Born-Oppenheimer approximation, Electronic, Vibrational and rotational spectrum of diatomic molecules, Selection rules, Frank-Condon principle,

Unit III **16 Hours**

Molecular Spectroscopy: Microwave and Infrared spectroscopy of di- and polyatomic molecules, normal coordinates and their symmetry (CO2), FT-IR instrumentation, Raman Effect, rotational and rotation- vibrational Raman transitions, nuclear spin effects, polarization of Raman lines. Vibronic spectroscopy of diatomic molecules, Franck-Condon factor, rotational fine structure

Unit IV **14 Hours**

Elementary particles: Classification of fundamental forces. Elementary particles and their quantum numbers (charge, spin, parity, isospin, strangeness, etc.). Gellmann-Nishijima formula. Quark model, baryons and mesons. C, P, and T invariance. Application of symmetry arguments to particle reactions. Parity non-conservation in weak interaction. Relativistic kinematics.

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

Suggested Readings

1. Modern Spectroscopy, J. M. Hollas, 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, Tata McGraw Hill, New Delhi (1994).
4. Principle of Fluorescence Spectroscopy, L. R. Lakowicz, 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).
7. Fundamentals of Molecular Spectroscopy, C. N. Banwell and E. M. McCash, (Tata, McGraw Hill Publishing Company Limited).
8. C.J. Foot, Atomic Physics (Oxford University Press, Oxford, U. K.) 2005.

Course Title: M.Sc. Project I
Paper Code: CCC.599
Invested Hours: 180

L	T	P	Cr
0	0	0	6

Course Objective and Learning Outcomes: The objective of project 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
Continuous Assessment		
1.	Review of literature and Bibliography	10
2.	Identification of gaps in knowledge	10
3.	Objective formulation	15
4.	Methodology	15
5.	Continuous evaluation of student by guide	30
Research Presentation		
6.	Presentation	20
	Total	100*

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)

***Evaluation Criteria:**
S or Satisfactory: >= 60
U or Unsatisfactory: < 60

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

Course Title: Introduction to Molecular Docking
Paper Code: CCC.559
Total Lectures: 15

L	T	P	Cr
1	0	0	1

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

- demonstrate various force field for biomolecular modeling
- execute various molecular docking methods
- identify the dynamics of structural transitions

which will help them to develop the molecular docking techniques in their further potential careers in academia and industry.

Course Content

Unit 1 **3 Hours**

Biomoleuclar structure and molecular recognition,

Unit 2 **4 Hours**

3D structure determination and molecular modeling,

Unit 3 **4 Hours**

Protein structure prediction, force fields for molecular dynamics simulation,

Unit 4 **4 Hours**

Different molecular docking methods, software's used in molecular docking.

Transactional Modes: Lectures; Problem solving; Self-learning.

Suggested Readings

1. Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo Molecular design : concepts and
applications Weinheim: Wiley-VCH, c2008
2. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
3. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley
International Publishers.
4. http://autodock.scripps.edu/faqs-help/manual/autodock-4-2-user-guide/AutoDock4.2_UserGuide.pdf

SEMESTER IV

Course Title: Electronic Structure Theory Lab (Practical)
Paper Code: CCC.573
Total Hours: 120

L	T	P	Cr
0	0	8	4

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 structure 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 surface generation.
8. Transition state calculations.

9. Absorption spectra study.
10. Calculations using solvent.
11. Thermochemistry study.
12. Post-HF based calculations
13. Studying potential energy surface.
14. Carrying of conformational analysis of large systems.
15. Model chemistry.
16. Study of NMR spectra
17. QM/MM 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: Enrich Chemistry Course - I
Paper Code: CCC.571
Total Hours: 30

L	T	P	Cr
2	0	0	2

Course Content

Unit I **8 Hours**

Chemical bonding in diatomics; elementary concepts of MO and VB theories; Huckel theory for conjugated π-electron systems. Chemical applications of group theory; symmetry elements; point groups; character tables; selection rules.

Unit II **7 Hours**

Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance – Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.

Unit III **8 Hours**

Chemical kinetics: Empirical rate laws and temperature dependence; complex reactions; steady state approximation; determination of reaction mechanisms; collision and transition state theories of rate constants; unimolecular reactions; enzyme kinetics; salt effects; homogeneous catalysis; photochemical reactions.

Unit IV **7 Hours**

Colloids and surfaces: Stability and properties of colloids; isotherms and

surface area; heterogeneous catalysis. Polymer chemistry: Molar masses; kinetics of polymerization.

Transactional Modes: Lectures; Problem solving; Self-learning.

Suggested Readings

1. Barrow, G. M. Physical Chemistry, 2007, Tata McGraw-Hill.
2. Kapoor, K. L. Text Book of Physical Chemistry, Volume 2-3,5, 2011, Macmillan.
3. Atkins, P. and De Paula, J. Atkins' Physical Chemistry. 2009, Oxford University Press.
4. McQuarrie, D. A. and Simon, J. D. Physical Chemistry: A Molecular Approach, 1998, Viva Books.
5. Moore, J. W. and Pearson, R. G. Kinetics and Mechanism, 1981, John Wiley and Sons.
6. Engel, T., Reid, P. and Hehre, W. Physical Chemistry, 2012, Pearson Education.
7. Rastogi, R. P. and Mishra, R. R. An Introduction to Chemical Thermodynamics, 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, 2012, Dover Publication Inc.
11. Hill, T. L. An Introduction to Statistical Thermodynamics, 1986, Dover Publications Inc.

Course Title: Enrich Chemistry Course - II
Paper Code: CCC.572
Total Hours: 30

L	T	P	Cr
2	0	0	2

Course Content

Unit I **5 Hours**

Organic reactive intermediates: Generation, stability and reactivity of carbocations, carbanions, free radicals, carbenes, benzynes and nitrenes.
Organic transformations and reagents: Functional group interconversion including oxidations and reductions; common catalysts and reagents (organic, inorganic, organometallic and enzymatic). Chemo, regio and stereoselective transformations.

Unit II **10 Hours**

Concepts in organic synthesis: Retrosynthesis, disconnection, synthons, linear and convergent synthesis, umpolung of reactivity and protecting groups.
Asymmetric synthesis: Chiral auxiliaries, methods of asymmetric induction –substrate, reagent and catalyst controlled reactions; determination of enantiomeric and diastereomeric excess; enantio-discrimination. Resolution – optical and kinetic.

Pericyclic reactions – electrocyclisation, cycloaddition, sigmatropic rearrangements and other related concerted reactions. Principles and applications of photochemical reactions in organic chemistry.

Unit III **5 Hours**

Concepts of acids and bases, Hard-Soft acid base concept, Non-aqueous solvents. Main group elements and their compounds: Allotropy, synthesis, structure and bonding, industrial importance of the compounds. Transition elements and coordination compounds: structure, bonding theories, spectral and magnetic properties, reaction mechanisms. Inner transition elements: spectral and magnetic properties, redox chemistry, analytical applications.

Unit IV **10 Hours**

Organometallic compounds: synthesis, bonding and structure, and reactivity. Organometallics in homogeneous catalysis. Cages and metal clusters.

Bioinorganic chemistry: photosystems, porphyrins, metalloenzymes, oxygen transport, electron- transfer reactions; nitrogen fixation, metal complexes in medicine. Characterisation of inorganic compounds by IR, Raman, NMR, EPR, Mössbauer, UV-vis, NQR, MS, electron spectroscopy and microscopic techniques.

Transactional Modes: Lectures; Problem solving; Self-learning.

Suggested Readings

1. Clayden, J., Greeves, N., Warren, S. and Wothers, P. Organic Chemistry, 2012, Oxford University Press.
2. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part A, 2002, Kluwer Academic Publishers.
3. Carey B. F. A., Sundberg R.J., Advanced Organic Chemistry Part B, 2007, Springer Science and Business Media Ltd.
4. Finar, I.L. Organic Chemistry Volume 1, 2012, Pearson Education UK.
5. Gilchrist, T.L. (1997). Heterocyclic Chemistry, 1997, Addison Wesley Longman Publishers, US.
6. Kalsi, P.S. Organic Reactions and Their Mechanisms. 2010, New Age International, New Delhi.
7. Morrison, R.T. and Boyd, R.N. Organic Chemistry, 2011, Prentice- Hall of India, New Delhi.
8. Smith, M. B. March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure, 2013, John Wiley & Sons.
9. Sykes, P. A Guide Book to Mechanism in Organic Chemistry, 1997, Prentice Hall.
10. Norman, R.O.C. and Coxon, J.M. Principles of Organic Synthesis, 1998, Nelson Thornes, Blackie Academic & Professional.
11. Cotton, F.A.; Wilkinson Advanced Inorganic Chemistry, 2007, John Wiley& Sons.
12. Huheey, J. E. Inorganic Chemistry: Principles of Structure and Reactivity, 2006, Dorling Kindersley (India) Pvt. Ltd.
13. Greenwood, N.N. and Earnshaw, A. Chemistry of the Elements, 2005 (reprinted), Butterworth-Heinemann, A division of Read Educational

& Professional Publishing Ltd.
14. Shriver, D.F.; Atkins, P.W. Inorganic Chemistry, 5th edition, 2010, Oxford University Press.
15. Dutta, R.L.; Syanal, A. Elements of Magnetochemistry, 1993, Affiliated East West Press.
16. Drago, Russell S. Physical Methods for Chemists, 1992, Saunders College Publishing.

Course Title: Advanced Molecular Simulation Lab
Paper Code: CCC.575
Total Hours: 120

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

Course Content

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: Advanced Statistical Mechanics and Molecular Reaction Dynamics
Paper Code: CCC.574
Total Lectures: 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 states of reactions

Course Content

Unit I **16 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 **14 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 **14 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 **16 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, (2008).
2. R. K. Pathria and P. D. Beale, Statistical mechanics, Elsevier, (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. A. H. Zewail, Femtochemistry-Ultrafast Dynamics of the Chemical Bond, World Scientific, New Jersey (1994).

Course Title: Biomolecular Structure Modeling
Paper Code: CCC.576
Total Lectures: 60

L	T	P	Cr
4	0	0	4

Learning Outcomes: On completion of the course the student should be able to:

- describe different types of protein–ligand interactions and characterise binding pockets
- use different search methods to find compounds with specific properties in large compound databases
- set up, perform and evaluate different virtual screening methods using large datasets
- account for and set up molecular dynamics simulations and free energy calculations

Course Content

Unit 1 **15 Hours**

Basics of Biomolecules: Principles of protein and nucleic acid structure: Primary, Secondary, Tertiary structure and Qaternary structure.

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

Unit 2 **15 Hours**

Protein tertiary structure modeling: Basic concepts, Protein folding and Energetics, Comparative modeling, Threading, Ab initio modeling, Modeling protein sidechains, CASP: A blind protein structure prediction competition, CAPRI, Protein Structure Initiative (PSI).

Unit 3 **15 Hours**

Introduction to drug designing, ADMET, drug metabolism, toxicity and pharmacokinetics, Identification and validation strategies. Drug Target classification, Design and development of combinatorial libraries for new lead generation.

Unit 4 **15 Hours**

Concept of Pharmacophore, Functional group considered as pharmacophore, Ehrlich's magnetic bullet, Fischer's Lock and Key, Structure-based drug design–'de novo' design methodologies 3D-database searching techniques, docking. QSAR

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

Suggested Readings

1. Grant, Guy H.; Richards, W. Graham Computational chemistry Oxford: Oxford Univ. Press, 1995
2. Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo Molecular design : concepts and applications Weinheim: Wiley-VCH, c2008

3. Andrew R.Leach Molecular Modelling Principles and applications . (2001) II ed . Prentice Hall.
4. Lednicer, D. "Strategies for Organic Drug Discovery Synthesis and Design"; (1998) Wiley International Publishers.
5. Gordon, E.M. and Kerwin, J.F "Combinatorial chemistry and molecular diversity in drug discovery" (1998) Wiley-Liss Publishers.

Course Title: Practicals in Biomolecular Structure Modeling
Paper Code: CCC.577
Total Hours: 120

L	T	P	Cr
0	0	8	4

Learning Outcomes: On completion of the course the student should be able to:

- identify different types of protein–ligand interactions and characterise binding pockets
- apply different search methods to find compounds with specific properties in large compound databases
- evaluate different virtual screening methods using large datasets
- devise and set up molecular dynamics simulations and free energy calculations

The following experiments should be conducted by the students:
A. Molecular Recognition
1. Prediction of Protein-ligand interaction sites
2. Prediction of Protein-protein interaction sites
3. Prediction of Protein-membrane interaction sites
4. Prediction of Protein-nucleic acid interaction sites
B. Docking
1. Protein Ligand Docking using
(i) Autodock
(ii) Vina
(iii) Dock
2. Protein-protein docking by HADDOCK or other similar methods
C. Modelling macromolecular structure
1. Homology modeling
2. *ab-initio* structure modeling

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

Suggested Readings
1. *Grant, Guy H.; Richards, W. Graham* Computational chemistry
Oxford: Oxford Univ. Press, 1995
2. *Schneider, Gisbert; Baringhaus, Karl-Heinz; Kubinyi, Hugo* Molecular design : concepts and applications
Weinheim: Wiley-VCH, c2008

Course Title: Bioinformatics for Transcriptomics and Metabolomics
Paper Code: LBI.574
Total Hours: 15

L	T	P	Cr
1	0	0	1

Learning Outcomes: On completion of the course the student should be able to:

- Identify to process the raw read file generated by Illumina sequencing.
- carry out the reference base expression estimation analysis
- learn alignment QC, visualization and differential expression studies

Course Content

Unit I **4 Hours**

Introduction to NGS techniques: Illumina (Solexa) sequencing, Roche 454 sequencing,

Unit II **4 Hours**

Ion torrent: Proton/PGM sequencing, SOLiD sequencing; sequence formats and quality.

Unit III **4 Hours**

Alignment of Next-Gen sequences to reference sequences, RNA-Seq analysis-Transcriptome mapping and differential expression: tools and pipeline.

Unit IV **3 Hours**

Introduction to metabolomics.

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

Suggested Readings

1. Shawn E. Levy and Richard M. Myers, "Advancements in Next-Generation Sequencing". Annu. Rev. Genom. Hum. Genet. 2016. 17:16.1–16.21
2. Beginner's Handbook of Next Generation Sequencing, Genohub
3. Next Generation Sequencing Methods and Protocols. Head, Steven R., Ordoukhanian, Phillip, Salomon, Daniel R

Course Title: M.Sc. Project-II
Paper Code: CCC.599
Total Hours: 180

L	T	P	Cr
0	0	0	6

Course Objective and Learning Outcomes: The objective of project 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
Continuous Assessment		
1.	Research work and Report writing	40
2.	Continuous evaluation of student by guide	30
Research Presentation		
3.	Presentation and defense of research work	30
	Total	100*

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)

***Evaluation Criteria:**

S or Satisfactory: >= 60
U or Unsatisfactory: < 60

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