COURSE STRUCTURE AND SYLLABUS

RECOMMENDED BY THE

BOARD OF STUDIES (CENTRE FOR COMPUTATIONAL SCIENCES)

FOR

MSc Chemistry (Computational Chemistry)

2015-16

Central University of Punjab
Bathinda-151001

Certificate

The Board of Studies of Centre for Computational Sciences certifies that the syllabus of MSc Chemistry (Computational Chemistry) has been designed to ensure maximal overlap with the CSIR-NET syllabus.

Prof. P. Ramarao **(Chairperson, BOS)**	Dr. Kousik Giri **(Member, BOS)**	Dr. Mahesh Kulharia **(Member. BOS)**
Dr. A. K. Dhawan **(Member, BOS)**	Er. S. S. Khurana **(Member, BOS)**	Dr. Sandeep Singh **(Member, BOS)**
Prof. Prasad V. Bharatam **(Member, BOS)**	Prof. Gursharan Singh **(Member, BOS)**	

Certificate

The Board of Studies of Centre for Computational Sciences certifies that the syllabus of MSc Chemistry (Computational Chemistry) has been designed in alignment with the Choice Based Credit System (CBCS) of UGC.

The percentage of foundation, core and elective courses for this programme are given below:

Course Type	Percentage of course type in the Programme	Percentage of course type required under CBCS
Foundation courses	14.6%	10-15%
Core Courses	58.3%	50-65%
Elective Courses	27.1%	25-35%

Prof. P. Ramarao
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(Member, BOS)

Programme Objective:

The objective of M. Sc. Chemistry (Computational Chemistry) Programme is that a student graduating after successful completion of the Programme shall be proficient in understanding the intricacies of relationship and interplay between Chemistry and Computational Sciences. This course is expected to enable the students to attain a Master's level understanding of Chemistry in general and Computational Chemistry in particular. In addition, based on the research training provided in this course, the students should be enabled to understand concurrent scientific literature, identify the knowledge lacunae, shortlist attainable objectives, design comprehensive methodology and carry out further research in higher degrees. In addition, extensive stress on logic based discipline would ensure development of scientific temperament among the students. Therefore graduated students of MSc Chemistry (Computational Chemistry) would be valuable asset for the nation by virtue of their scientific abilities. The student can expect successful career/employment in academic / research / industry by undertaking this course. A special effort has been made to enable the student clear national level tests for teaching ability and research fellowships especially, CSIR-NET.

CENTRAL UNIVERSITY OF PUNJAB, BATHINDA – 151001
Centre for Computational Sciences
M.Sc. Chemistry (Computational Chemistry)
Course Structure and Syllabus as per Choice Based Credit System (CBCS)

Semester I

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	% Weightage				E
								A	B	C	D	
1	CHM.501	Computer Applications	F	2	0	0	2	25	25	25	25	50
2	CHM.502	Inorganic Chemistry-I	C	4	0	0	4	25	25	25	25	100
3	CHM.503	Organic Chemistry-I	C	4	0	0	4	25	25	25	25	100
4	CHM.504	Physical Chemistry-I	C	4	0	0	4	25	25	25	25	100
5	CHM.505	Spectral Analysis	C	4	0	0	4	25	25	25	25	100
6	CHM.506	Organic Chemistry Practical	C	0	0	4	2	-	-	-	-	100
7	CHM.507	Inorganic Chemistry Practical	C	0	0	4	2	-	-	-	-	50
8		Inter-Disciplinary Elective	E	2	0	0	2	25	25	25	25	50
				20	0	8	24					600
Interdisciplinary Course for other Centres												
	CSC.501	Chemistry without test tube	E	2	0	0	2	25	25	25	25	50

Semester II

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	% Weightage				E
								A	B	C	D	
1	CHM.508	Inorganic Chemistry II	C	4	0	0	4	25	25	25	25	50
2	CHM.509	Organic Chemistry II	C	4	0	0	4	25	25	25	25	50
3	CHM.510	Physical Chemistry II	C	4	0	0	4	25	25	25	25	100
4	CSC.502	Quantum Chemistry-I	C	4	0	0	4	25	25	25	25	100
5	CHM.512	Physical Chemistry Practical	C	0	0	4	2	-	-	-	-	100
6	CSC.503	Molecular Spectroscopy	C	4	0	0	4	25	25	25	25	50
7		Interdisciplinary Elective	E	2	0	0	2	25	25	25	25	50
				22		16	24					600

Semester III

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	% Weightage				E
								A	B	C	D	
1	CSC.601	Computational Chemistry	E	4	0	0	4	25	25	25	25	100
2	CSC.602	Research Methodology	F	2	0	0	2	25	25	25	25	50
3	CSC.603	Dissertation	C	0	0	12	6	-	-	-	-	150
4	CSC.604	Elective Course –I	E	4	0	0	4	25	25	25	25	100
5	CSC.605	Computer Programming and Scripting	F	4	0		4	25	25	25	25	100
6	CSC.606	Computer Programming and Scripting Lab	F	0	0	8	4	-	-	-	-	100
				14	0	20	24					600
Elective Course-I												
	CSC.604	Density Functional Theory	E	4	0	0	4	25	25	25	25	100

Semester IV

S. No.	Paper Code	Course Title	Course Type	L	T	P	Cr	% Weightage				E
								A	B	C	D	
1	CSC.607	Fundamentals of Molecular Simulations	E	4	0	0	4	25	25	25	25	100
2	CSC.608	Molecular Simulations Lab	E	2	0	0	2	-	-	-	-	50
3	CSC.609	Elective Course-II	E	4	0	0	4	25	25	25	25	100
4	CSC.610	Elective Course-III	E	4	0	0	4	25	25	25	25	100
5	CSC.599	Seminar	F	-	-	4	2	-	-	-	-	50
6	CSC.611	Dissertation Research	C	-	-	16	8	25	25	25	25	200
				14	0	0	24					600
Elective Course-II												
1	CSC.609	Modeling Polymeric Materials	E	4	0	0	4	25	25	25	25	100
Elective Course-III												
1	CSC.610	Computational Chemistry Lab	4	4	0	0	4	-	-	-	-	100

A: Continuous Assessment: Subjective by enlarge
B: Mid-Term Test-1: Based on Objective Type and Subjective Test
C: Mid-Term Test-2: Based on Objective Type and Subjective Test
D: End-Term Exam (Final): Based on Objective Type Tests; **E: Total Marks**
C: Core; E: Elective and Interdisciplinary; F: Foundation; L: Lectures; T: Tutorial; P: Practical; Cr: Credits.

Semester I

Objective and Expected Learning Outcomes: The course structure of semester I of this Programme is designed to ensure complete overlap with courses taught to students of M. Sc. Chemical Sciences and M. Sc. Chemical Sciences (Medicinal Chemistry). Thus, the first semester includes courses in inorganic, organic, physical chemistry and some interdisciplinary courses and is designed to provide breadth of knowledge in the discipline of Chemistry. The breadth knowledge gained in this semester will help students better understand the interdisciplinary area of Computational Chemistry. The list of courses to be taught in this semester is provided below, and is adapted from the Course structure of M. Sc. Chemical Sciences programme currently running in the Centre for Computational Sciences of CUPB.

Course Title: Computer Applications
Paper Code: CHM.501
Total Lectures: 36

L	T	P	Credits	Marks
36	0	0	2	50

Objective and Learning outcomes: The objective of this course is to provide an idea of the basic computer applications. After completing this course, the students are expcted to have an understanding of the basic understanding of applications of computers in routine academic work.

Unit I

Fundamentals of computers: Parts of computers, Hardware, BIOS, Operating systems, Binary system, Logic gates and Boolean algebra.

Application software: Spreadsheet applications, Word-processing applications, Presentation applications, Internet browsers, Reference Management, and Image processing applications.

Unit II

Computer language: Basic DOS commands, AutoHotKey scripting language, HTML and basic structure of a webpage, Designing websites.

World wide web: Origin and concepts, Latency and bandwidth, Searching the internet, Advanced web-search using Boolean logic, Cloud computing.

ESSENTIAL BOOKS

1. Gookin, D. (2007). *MS Word 2007 for Dummies*. Wiley.
2. Harvey, G. (2007). *MS Excel 2007 for Dummies*. Wiley.
3. Johnson, S. (2009). *Windows 7 on demand*. Perspiration Inc.
4. Norman, G. and Streiner, D. (3rd edn) (2008). *Biostatistics: The Bare Essentials*. Decker Inc., Canada.
5. Sokal, R.R. and Rohlf, F.J. (1994). *Biometry: The Principles and Practices of Statistics in Biological Research*, W.H. Freeman and Company, New York.

Thurrott, P. and Rivera, R. (2009). *Windows 7 Secrets*. Wiley

Course Title: Inorganic Chemistry-I
Paper Code: CHM.502
Total Lectures: 72

L	T	P	Credits	Marks
72	0	0	4	100

Objective and Learning Outcomes: The objective of this course is that students learn the principles of inorganic chemistry, which is a fundamental branch of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in inorganic chemistry.

Unit I **12 hrs**

Metal-Ligand Equilibria in Solution

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

Unit II **20 hrs**

Symmetry Elements and Molecular Orbital Theory

Symmetry elements, symmetry operations and their matrix representation, group postulates and types, multiplication tables, point group determination, determination of reducible and irreducible representations, character tables, construction of character tables for C2v, C3v, use of symmetry in obtaining symmetry of orbitals in molecules, qualitative splitting of s, p, d, f orbitals in octahedral, tetrahedral and square planar fields using character tables and without the use of character tables. Ligands symmetry orbitals and metal orbitals involved in molecular orbitals formation in octahedral complexes, MOEL diagrams for octahedral tetrahedral and square planar complexes showing σ and π bonding in transition metal complexes.

Unit III **20 hrs**

Crystal Fields Splitting

Spin-spin, orbital-orbital and spin orbital coupling, LS and jj coupling schemes, determination of all the spectroscopic terms of pn, dn ions, determination of the ground state terms for pn, dn, fn ions using L.S. scheme, determination of total degeneracy of terms, order of interelectronic repulsions and crystal field strength in various fields, two type of electron repulsion parameters, 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 (with help of the character table). Splitting patterns of and G, H and I terms. Strong field configurations, transition from weak to strong crystal fields, evaluation of strong crystal field terms of d2 configuration in octahedral and tetrahedral crystal fields (using group theory), construction of the correlation energy level diagrams of d2 configuration in octahedral field, study of energy level diagrams for higher configurations, selection rules of electronic transitions in transition metal complexes, their proof using group theory, relaxation of the selection rule in Centro symmetric and non-centro

symmetric molecules, Orgel diagrams, Tanabe Sugano diagrams, calculation of 10Dq and B with use of Orgel and Tanabe Sugano diagrams, quenching of orbitals angular momentum by ligand field.

Unit IV **20 hrs**

Electronic Spectra of Transition Metal Complexes

Variation of the Racah parameter, nephlauxetic effect -central field covalency, symmetry restricted covalency, differential radial expansion, spectrochemical series, band intensities, factors influencing band widths, 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 statesmixing, first order and second order Zeeman effects, Spin paired and spin-free equilibria in complexes magnetic properties of polynuclear complexes involving OH, NH2 and CN bridges.

ESSENTIAL BOOKS:

1. Cotton, F.A.; Wilkinson *Advanced Inorganic Chemistry*, 6th edition, John Wiley& Sons, 1999.
2. Huheey, James E. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th edition, Harper Collins College Publishers, 1993.
3. Greenwood, N.N. and Earnshaw, A. *Chemistry of the Elements*, 2nd edition, Butterworth-Heinemann, A division of Read Educational & Professional Publishing Ltd., 2001.
4. Lever, A.B.P. *Inorganic Electronic Spectroscopy*, 2nd edition, Elsevier Science Publishers B.V., 1984.
5. Carlin, Richard L. and Duyneveldt, A.J.Van *Magnetic Properties of Transition Metal Compounds*, Inorganic Chemistry Concepts 2, Springerverlag New York Inc., 1977.
6. Miessler,G. L.and Tarr, D. A. *Inorganic Chemistry,*Pearson Education, 3rd edition.
7. Figgis,B.N. *Introduction to Ligand Field,* Wiley Eastern.
8. Drago,R.S. *Physical Method in Chemistry,* W.B. Saunders Company.
9. Shriver, D.F.; Atkins, P.W. *Inorganic Chemistry*, 1st edition, Oxford University Press, 2006.
10. Earnshaw, A. *Introduction to Magnetochemistry*, Academic Press, 1968.
11. Dutta, R.L.; Syanal, A. *Elements of Magneto chemistry*, 2nd edition, Affiliated East West Press, 1993.
12. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.

Course Title: Organic Chemistry-I
Paper Code: CHM.503
Total Lectures: 72

L	T	P	Credits	Marks
4	0	0	4	100

Objective and Learning Outcomes: The objective of this course is that students learn the principles of organic chemistry, which is a fundamental branch 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 organic chemistry.

Unit I **22hrs**

Stereochemistry: IUPAC nomenclature of organic molecules, Elements of symmetry, chirality, Projection formulae [Fly wedge, Fischer, Newman and Saw horse], Configurational and conformational isomerism in acyclic and cyclic compounds; stereogenicity, stereoselectivity, enantioselectivity, diastereoselectivity, racemic mixture and their resolution, configurational notations of simple molecules, DL and RS 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 the course of rate of reactions, effect of conformation on reactivity, conformation of sugars, strain due to unavoidable crowding, geometrical isomerism, *cis–trans* and E-Z conventions, methods of inter-conversion of E and Z isomers, determination of configuration by physical and chemical methods.

Unit II **18 hrs**

Aliphatic nucleophilic subsitution reaction: The SN2, SN1, mixed SN1 and SN2 and SET mechanism, The SNi 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 between SN1 and SN2 mechanism.

Aromatic nucleophilci substitution: The SNAr, benzyne and SN1 mechanism, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Aliphatic electrophilic substitution: Bimolecular mechanisms SE2 and SE1 mechanism, electrophilic substution accompanied by double bond shifts, effect of substrates, leaving groups and the solvent polarity on the reactivity.

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, Diazonium coupling, Vilsmeir reaction, Gatterman-Koch reaction.

Unit III **16 hrs**

Elimination reactions: The E2, E1 and E1cB mechanisms and their spectrum, orientation of the double bond, reactivity 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, Regio- and chemoselectivity, orientation and reactivity, hydroboration, alkylation, epoxidation and hydroxylation, addition of halogen polar reagents to alkenes.

Unit IV **16 hrs**

Addition to carbon-hetero multiple bonds: Reactivity of carbonyl group, homologation and dehomologation of carbonyl compounds, nucleophilic addition of hetero-atoms (N,O,S), conjugate addition reactions, acylation of carbonyl carbon, carbonyl cyclizations and cleavages, carboxylic acids and derivatives, decarboxylation reactions, addition of Grignard, organozinc and organolithium reagents to carbonyl and unsaturated carbonyl compounds, mechanism of condensation reactions involving enolates-Aldol, Knoevenagel, Claisen, Mannich, Benzoin, Perkin and Stobbe reactions, hydrolysis of esters and amides, ammonolysis of esters.

ESSENTIAL BOOKS:

1. Finar, I.L., (2003). *Organic Chemistry Vol. 1*. Pearson Education, 4th edition.
2. Mc Murry J., *Organic Chemistry***,** Asian Book Pvt. Ltd, 8th edition, New Delhi
3. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
4. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism***,** Narosa Publishing House (P) Ltd., 4th edition, New Delhi-110002.
5. Bansal, R. K., (2010). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Bansal R.K., (2010). *Organic Reaction Mechanism*, New Age International (P) Ltd., New Delhi.
7. Kalsi, P.S., (2010). *Organic Reactions and Their Mechanisms*. New Age International Pub., 3rd edition, New Delhi.
8. Kalsi, P.S., (2010). *Stereochemistry: Conformation and Mechanism*, New Age International (p) Ltd. New Delhi.
9. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, New York.
10. Morrison, R.T., Boyd, R.N. (2011). *Organic Chemistry*, Prentice- Hall of India, 6th edition, New Delhi.
11. Mukherjee, S.M. Singh, S.P., (2009). *Reaction Mechanism in Organic Chemistry.* Macmillan India Ltd., 3rd edition, New Delhi.
12. Robert and Casereo, (1977). *Basic principle of Organic Chemistry***,** Addison-Wesley, 2nd edition.
13. Solomn, C.W.G, Fryble, C.B. (2009). *Organic Chemistry*. John Wiley and Sons, Inc., 10th edition.
14. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, 6th edition.
15. Eliel, E. L., & Wilen, S. H. (2008). *Stereochemistry of organic compounds*. John Wiley & Sons.

Course Title: Physical Chemistry-I
Paper Code: CHM.504
Total Lectures: 72

L	T	P	Credits	Marks
4	0	0	4	100

Objective and Learning Outcomes: The objective of this course is that students learn the principles of physical chemistry, which is a fundamental branch of Chemistry. A thorough understanding of the content of this course will prepare the students to understand how the computational techniques can be applied to study problems in physical chemistry.

Unit I **18 hrs**

Surface Chemistry and Catalysis: Bimolecular surface reactions-reaction between a gas molecule and adsorbed molecule, reaction between two adsorbed molecules, inhibition and activation energy of such reactions. Catalytic activity at surfaces, transition state theory of surface reactions: rates of chemisorption and desorption, unimolecular and bimolecular surface reaction, comparison of homogeneous and heterogeneous reaction rates, surface heterogeneity, lateral interaction. Adsorption of solids, Gibbs adsorption isotherm, BET adsorption isotherm: estimation of surface area of solids.

Unit II **18 hrs**

Electrochemistry: Nernst equation, redox systems, electrochemical cells; Debye-Huckel theory; electrolytic conductance–Kohlrausch's law and its applications; ionic equilibria; conductometric and potentiometric titrations.
Solid State: Crystal structures; Bragg's law and applications; band structure of solids.

Unit III **16 hrs**

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; homogeneous catalysis; photochemical reactions.

Unit IV **20 hrs**

Polymer Chemistry: Classification of polymers, kinetics of polymerizations, Molecular weight, molecular weight distribution and its control in polymerization. Copolymerization, polymerization techniques and control of polymer structure and properties and its applications.
Nuclear Chemistry: Classification of nuclides, Nuclear stability, Atomic energy, Types of nuclear reactions-fission and fusion, Conservation in nuclear reactions-linear momentum and mass-energy, Reaction cross-section, Bohr's compound nucleus theory of nuclear reaction.

ESSENTIAL BOOKS:

1. Physical Chemistry, G. M. Barrow, TATA MCGRAW-HILL, 2007.
2. Text Book of Physical Chemistry, K. L. Kapoor, MACMILLAN, 2006.
3. Physical Chemistry, A. W. Atkins, W. H. Freeman, and Company, 1997.
4. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon,Viva Books, 2011.
5. Kinetics and Mechanism, J. W. Moore, and R. G. Pearson, John Wiley and Sons, 1981.

6. Physical Chemistry, R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Wiley-Interscience Publication, 2013.
7. Physical Chemistry, T. Engel, and P. Reid, Prentice-Hall, 2012.

Course Title: Spectral Analysis
Paper Code: CHM.505
Total Lectures: 72

L	T	P	Credits	Marks
4	0	0	4	100

Objective and Learning Outcomes: The objective of this course is that students get a basic understanding of how to analyze the spectra obtained from different spectroscopic techniques, that are relevant to the discipline 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 molecular spectroscopy.

Unit I **18 hrs**

UV-Visible spectroscopy: Principle of UV-Visible Spectroscopy, Chromophores and their interaction with UV-visible radiation and their utilization in structural, qualitative and quantitative analysis of drug molecules. Woodward-Fieser rule, solvent effects, stereochemical effect.

Infrared Spectroscopy: Infrared radiation and its interaction with organic molecules, vibrational mode of bonds, instrumentation and applications, effect of hydrogen bonding and conjugation on absorption bands, interpretation of IR spectra. FTIR.

Unit II **18 hrs**

Nuclear magnetic resonance spectroscopy: Magnetic properties of nuclei, Field and precession, Chemical shift concept, Isotopic nuclei, Reference standards and solvents. ^{1}H- NMR spectra, Chemical shifts, Spin spin coupling, Coupling constants, Integration of signals, Interpretation of spectra, Decoupling, double resonance and shift reagent methods, Long range coupling, Resonance of other nuclei e.g. ^{19}F, ^{15}N, ^{31}P.

Unit III **18 hrs**

Principles of FT-NMR with reference to ^{13}C NMR, Free induction decay, Average time domain and frequency domain signals, Spin-spin and spin-lattice relaxation phenomenon, Nuclear Overhauser enhanced (NOE), ^{13}C NMR spectra, their interpretation and application. APT and DEPT techniques, Principle of 2-D NMR, Correlation spectroscopy (COSY) Homo COSY (^{1}H-^{1}H COSY), Hetro COSY (^{1}H-^{13}C COSY, HMQC), long range ^{1}H-^{13}C COSY (HMBC), NOESY, DEPT and 2D INADEQUATE experiments and their application, Solid-state NMR.

Unit IV **18 hrs**

Mass spectrometry: Basic principles and brief outline of instrumentation, Ion formation, molecular ion, metastable ion, Mc Lafferty rearrangement, Nitrogen rule, fragmentation process in relation to molecular structure and functional groups. Relative abundance of isotopes, chemical ionization, FAB, ESI and MALDI other recent advances in mass spectrometry.

ESSENTIAL BOOKS:

1. Banwell, C.N.; McCash, E. M. (2000). *Fundamentals of molecular spectroscopy*, Tata McGraw-Hill, New Delhi.
2. Dyer, J.R. (2009). *Application of Absorption Spectroscopy of Organic Compounds*, Publisher: Phi Learning.
3. Kalsi, P.S. (2004). *Spectroscopy of Organic Compounds*, New Age International Ltd.
4. Kemp, W. (1991). *Organic spectroscopy*, ELBS London.
5. Khopkar, S.M. (2007). *Basic Concepts of Analytical Chemistry*, New Age International Pvt Ltd.

6. Melinda J.D., (2010). *Introduction to solid NMR Spectroscopy*, Wiley India Pvt Ltd
7. Mendham, J.; Denney, R.C.; Barnes, J. D.; Thomas, M. J. K. (2003). *Vogel's Textbook of Quantitative Chemical Analysis*, Pearson Education Pvt. Ltd., New Delhi.
8. Pavia, D.L.; Lampman, G. M. (2010). *Introduction to Spectroscopy*, G. S. Kriz, Harcourt College, NY.
9. Popov, A.I.; Halenga, K. (1991). *Modern NMR techniques and their Applications*, Marcel Deckker.
10. Silverstein, R.M. (2006). *Spectrometric Identifications of Organic Compound***s**, John Wiley.
11. Skoog, D.A.; West, D.M.; Holler, F.J.; Crouch, S.R. (2004). *Fundamental of Analytical Chemistry*, Saunders College Publishing, New York.
12. Willard, H.H.; Merrit, L.L.; Dean, J.A.; Settle, F.A. (2001). *Instrumental methods of analysis*, CBS Publishers and Distributors.
13. Williams, D.H.; Fleming, I. (2004). *Spectroscopy Methods in Organic Chemistry*, Tata McGraw-Hill Publishing Co. Ltd., New Delhi.

Course Title: Organic Chemistry-Practical
Paper Code: CHM.506
Total Lectures: 36

L	T	P	Credits	Marks
-	0	4	2	50

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

A. **Techniques**: (At least One Practical of Each Technique)

Crystallization, Fractional Crystallization, Sublimation, Distillation, Fractional Distillation, Steam Distillation, Vacuum Distillation, Column Chromatography, Thin Layer Chromatography (Purity would be checked by m. p. and mixed m. p.).

B. **Preparation of Derivatives**: (Each Derivative of two Compounds) Oxime, 2, 4-DNP, Acetyl, Benzoyl, Semicarbazone, Anilide, Amide, Aryloxyacetic acid.

C. Preparations: Single Stage (Any 15)

1 Cyclohexanone to Adipic acid
2 Benzophenone to Benzhydral
3 Chlorobenzene to 2,4-Dinitrochlorobenzene
4 2,4-Dinitrochlorobenzene to 2,4-Dinitrophenol
5 Acetoacetic ester to 1-Phenyl-3-methyl-5 pyrazolone
6 Benzaldehyde to Cinnamic acid
7 4-Chlorobenzaldehyde to 4-Chlorobenzoic acid + 4-Chlorobenzyl alcohol
8 Benzene to β-Benzoyl propionic acid
9 Benzaldehyde to Dibenzylidene acetone
10 p-Aminobenzoic acid to p-Chlorobenzoic acid
11 N,N-Dimethylaniline to 4-Formyl-N, N-dimethyl aniline
12 Benzophenone to Benzpinacol
13 p-Nitrotoluene to p-Nitrobenzoic acid
14 Anisole to 2,4-Dinitroanisole
15 Phthalic anhydride to phthalimide
16 Phthalimide to Anthranilic acid
17 Acetanilide to p-Bromoacetanide
18 p-Bromoacetanide to p-Bromoaniline
19 m-Dinitrobenzene to m-Nitroaniline
20 Synthesis of Phenytoin

D. Use of Computer - Chem Draw-Sketch, ISI – Draw: Draw the structure of simple aliphatic, aromatic, heterocyclic organic compounds with substituents. Get the correct IUPAC name and predict the UV, IR and ^{1}H-NMR signals.

E. Demonstration of Stereochemical aspects of the compounds through molecular models.

ESSENTIAL BOOKS:

1. Harwood, L.M., Moody, C.J. *Experimental Organic Chemistry*, 1st edition, Blackwell Scientific Publishers, 1989.
2. Vogel, A.I. *Text Book of Practical Organic Chemistry*, ELBS, IVth edition, Longman Group Ltd.,1978.
3. Mann, F.G.; Saunders, B.C. *Practical Organic Chemistry*, 4th edition, New Impression, Orient Longman Pvt. Ltd., 1975.
4. Leonard, J.; Lygo, B. *Advanced Practical Organic Chemistry*, Chapman and Hall, 1995.
5. Armarego, W. L., & Chai, C. (2012). *Purification of laboratory chemicals*. Butterworth-Heinemann.
6. Young, J. A. (Ed.). (Latest Edition). *Improving safety in the chemical laboratory: a practical guide*. Wiley.

Course Title: Inorganic Chemistry Practical
Paper Code: CHM.507

L	T	P	Credits	Marks
-	0	4	2	50

Total Lectures: 36

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

Gravimetric Estimation

1. Determination of Ba^{2+} as its chromate.
2. Estimation of lead as its lead sulfate.
3. Estimation of Nickel (II) as its nickel dimethyl glyoximate.
4. Estimation of Cu^{2+}as cuprousthiocyanate.

Precipitation Titrations

1. $AgNO_3$ standardization by Mohr's method.
2. Volhard's method for Cl^- determination.
3. Determination of ammonium / potassium thiocyanate.

Oxidation-Reduction Titrations

1. Standardization of $KMnO_4$with sodium oxalate and determination of Ca^{2+} ion.
2. Standardization of ceric sulphate with Mohr's salt and determination of Cu^{2+}, NO_2^- and $C_2O_4^{-2}$ ions.
3. Standardization of $K_2Cr_2O_7$ with Fe^{2+} and determination of Fe^{3+} (Ferric alum)
4. Standardization of hypo solution with potassium iodate / $K_2Cr_2O_7$ and determination of available Cl_2 in bleaching powder, Sb^{3+} and Cu^{2+}.
5. Determination of hydrazine with KIO_3 titration.

ESSENTIAL BOOKS:

1. Pass, G.; Sutcliffe *Practical Inorganic Chemistry*, 1st edition, Chapmann and Hall Ltd., 1968.
2. Jolly, W.L. *Synthetic Inorganic Chemistry*, 2nd edition, Prentice Hall, Inc., 1961.
3. Nakamoto, Kazuo *Infrared and Raman Spectra of Inorganic and Coordinatio Compounds: Part A and B*, 5th edition, John Wiley and Sons, 1997.
4. Mendham, J; Denney, R.C.; Barnes, J.D.; Thomas, M. *Vogel's Textbook of Quantitative Chemical Analysis*, 6th edition, Pearson Education, Ltd., 2000.
5. Svehla,G. and Sivasankar,B.*Vogel's Qualitative Inorganic Analysis (revised)*,Pearson, 7th edition, 1996.

Interdisciplinary Courses (*recommended)

Course Title: *Mathematics for Chemists
Paper Code:
Total Lectures: 36

L	T	P	Credits	Marks
36	0	0	2	50

Objective and Learning Outcomes: This course is intended for those students who have not studied Mathematics in their Bachelor's degree. After taking this course, the students are expected to gain basic understanding of mathematical techniques, that are of paramount important in understanding subsequent courses including, but not limited to quantum chemistry I and electronic structure methods.

Unit I **9 hrs**

Matrices, Operations on Matrices, Determinants, Properties of determinants, Singular and nonsingular matrices, Adjoint and Inverse of a matrix, Rank of Matrix, The solution of linear equations Basic idea of linear transformation, orthogonal matrices and orthogonal transformations, Symmetry operations, The Eigen value problem, Properties of the Eigen vectors, Matrix Diagonalization

Unit II **9 hrs**

Limit and continuity, Differentiation from first principle, Differentiation by rule, Implicit functions, Logarithmic differentiation, successive differentiation Stationary points, Linear and angular motion. Integral as anti-derivative. Integration by substitution, by partial fractions and by parts. The method of partial fractions, parametric differentiation of integrals Definite integral and its properties. Areas of bounded regions Reduction formulas, rational integrands. Static properties of matter.

Unit III **9 hrs**

Basic concepts, Scalar product, Vector product, Vector differentiation, Arc length. Line, Surface and Volume integrals. The gradient, divergence and curl. The Del operator. Green's, Gauss' and Stokes' theorems (statements only)

Unit IV **9 hrs**

Permutation and Combination: Idea of Factorial notation for natural numbers, Fundamental principle of counting, basic concept of Permutation, Basic concept of Combination
Probability and probability theorems**:** introduction to probability, addition theorem of probability, multiplication theorem of probability.

ESSENTIAL BOOKS:

1. Steiner, E. *The Chemistry Mathematics*, 1st edition, Oxford University Press.
2. Doggett; Sucliffe *Mathematics for Chemistry*, 1st edition, Longman, 2003.
3. Daniels, F. *Mathematical Preparation for Physical Chemistry*, McGraw Hill.
4. Hirst, D.M. *Chemical Mathematics*, Longman.
5. Barrante, J. R. *Applied Mathematics for Physical Chemistry*, 3rd edition, Prentice Hall, 2004.
6. Tebbutt *Basic Mathematics for Chemists*, 1st edition, John Wiley, 1994
7. Dence,Joseph B.*Mathematical Techniques in Chemistry*, Wiley, 1975.
8. Narayan,Shanti andMittal,P. K. *A Text Book of Matrices*, S. Chand & Co. Ltd., Reprint 2002.

Course Title: *Biology for Chemists
Paper Code:

L	T	P	Credits	Marks
36	0	0	2	50

Total Lectures: 36

Objective and Learning Outcomes: This course is intended for those students who have not studied Life Sciences in their Bachelor's degree. After taking this course, the students are expected to gain basic understanding of life processes in general, including biomolecular structure and functions. This course will help students break psychological barriers into a discipline not studied earlier in detail on one hand, and better prepare the students to undertake interdisciplinary research on the other hand.

Unit I **9 hrs**

Cell Structure and Functions:

Structure of prokaryotic and eukaryotic cell, intracellular organelles and their functions, comparison of plant and animal cells. Overview of metabolic processes –catabolism and anabolism. ATP-the biological energy currency. Origin of life – unique properties of carbon, chemical evolution and rise of living systems. Introduction to biomolecules,
building blocks of bio-macromolecules.

Unit II **9 hrs**

Fatty acids, essential fatty acids, structure and function of triacylglycerols, glyerophosphplipids, cholesterol, bile acids, prostaglandins, lipoproteins-composition and function, role in atherosclerosis. Properties of lipid aggregates micelles, bilayers, liposomes and their possible biological functions. Bioligical membrans. Fluid mosaic model of membrane structure. Lipid metabolism - beta oxidation of fatty acid.

Unit III **9 hrs**

Amino-acids, Peptides and Proteins:

Chemical and enzymatic hydrolysis of proteins to peptides, amino acid sequencing. Secondary structure of proteins forces responsible for holding of secondary structures. Alpha helix, Beta sheets, secondary structure, triple helix structure of collagen. Tertiary structure of protein-folding and domain structure. Quaternary structure. Amino acid metabolism- degradation and biosynthesis of amino acids, sequence determination chemical enzymatic mass spectral, racemization detection. Chemistry of oxytocin and tryptophan releasing hormone.

Unit IV **9 hrs**

Nucleic Acids:

Purines and pyrimidines bases of nucleic acids, base pairing via H-bonding. Structure of ribonucleic acids RNA and deoxyribonucleic acids DNA ,double helix model of DNA and forces responsible for holding it. Chemical and enzymatic hydrolysis of nucleic acids.The chemical basis for hereditary, an overview of replication of DNA, transcription, translation and genetic code. Chemical synthesis of mono and trinucleoside

ESSENTIAL BOOKS:

1. Lehninger, A.L. *Principles of Biochemistry,* Worth Publishers.
2. Stryer, L. *Biochemistry*, W.H. Freeman.
3. Rawn, J. David *Biochemistry*, Neil Patterson.
4. Voet; Voet *Biochemistry*, John Wiley.
5. Conn, E.E.; Stumpf, P. K. *Outlines of Biochemistry*, John Wile

Interdisciplinary courses for other Centres

Course Title: Chemistry without Test Tube (ID)
Paper Code: CSC.501
Total Hours: 36

L	T	P	Credits	Marks
36	0	0	2	50

Objective and Learning Outcomes: This course is intended for Science students from other centres of CUPB. Starting from high school level Chemistry as a background, this course will help the students understand how Chemistry concepts are understood and appreciated using theoretical and Computer models.

Unit I **9 hrs**

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 **9 hrs**

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 **9 hrs**

Lone pairs of electrons: Why are Not all electrons involved in bonding? What is a lone pair? Shapes of the simple molecules.

Organic molecules with multiple bonds: Double and triple bonds, ethene and methanal, reactivity of a double bond.

Diatomics with multiple bonds: N2, CO, O2

Dative Bonds: Solvation, reactive lone paire

Delocalized electronic substructures: The benzene molecule, delocalized electrons.

Unit IV **9 hrs**

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

ESSENTIAL BOOKS:

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

Semester II

Objective and Expected Learning Outcomes: The course structure of semester II of this Programme is designed to ensure maximum overlap with courses taught to students of M. Sc. Chemical Sciences and M. Sc. Chemical Sciences (Medicinal Chemistry). This semester includes advanced courses in inorganic, organic, physical chemistry and some interdisciplinary courses and is designed to provide breadth of knowledge in the discipline of Chemistry. In addition to these courses, two courses for paramount relevance to students of Computational Chemistry, viz. Quantum Chemistry I (which is common with students of M. Sc. Chemical Sciences) and Molecular Spectroscopy will prepare the students towards more advanced Computational Chemistry courses to be taken in Semester III and IV. In addition, the breadth knowledge gained in this semester will help students better understand the interdisciplinary area of Computational Chemistry. The list of courses to be taught in this semester is provided below, some of which are adapted from the Course structure of M. Sc. Chemical Sciences programme currently running in the Centre for Computational Sciences of CUPB.

Course Title: Inorganic Chemistry-II

L	T	P	Credits	Marks

Paper Code: CHM.508

4	1	0	4	100

Total Lectures: 72

Objective and Learning Outcomes: The objective of this course is that students learn the advanced topics in inorganic chemistry, and gain depth knowledge in this fundamental branch of Chemistry. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in inorganic chemistry.

Unit I **22 hrs**

Reaction Mechanisms of Transition Metal Complexes

Introduction, ligand replacement reactions, classification of mechanisms, Water exchange rates, formation of complexes from aqueous ions, catanation, reaction, aquation and base hydrolysis attack on ligands, reactions, of square planar complexes, mechanism of ligand displacement reactions; metal carbonyl reactions, reactions of binuclear carbonyls, associative reactions, species with 17 electron, electron transfer processes outer and inner sphere. The Marcus theory, doubly bridged inner-sphere transfer, other electron transfer reactions; two electron transfers, Non-complementary reaction, Ligand exchange via electron exchange, reductions by hydrated electrons, stereochemical non-rigidity, stereochemically non-rigid coordination compounds, Trigonal bipyramidal molecules, systems with coordination number six or more, isomerization and recombination's, tris chelate complexes, metal carbonyl scrambling cluster, rotation within Co shells.

Unit II **15 hrs**

Higher boranes, carboranes, metallobranes and metallocarboranes, metal carbonyl and halide clusters, compounds with metal-metal multiple bonds.

Unit III **15 hrs**

Metal Complexes

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 dioxygen complexes, tertiary phosphine as ligand.

Unit IV **20 hrs**

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.

ESSENTIAL BOOKS:

1. Cotton, F.A.; Wilkinson *Advanced Inorganic Chemistry*, 6th edition, John Wiley& Sons, 1999.
2. Huheey, James E. *Inorganic Chemistry: Principles of Structure and Reactivity*, 4th edition, Harper Collins College Publishers, 1993.
3. Greenwood, N.N. and Earnshaw, A. *Chemistry of the Elements*, 2nd edition, Butterworth-

Heinemann, A division of Read Educational & Professional Publishing Ltd., 2001.
4. Lever, A.B.P. *Inorganic Electronic Spectroscopy*, 2nd edition, Elsevier Science Publishers B.V., 1984.
5. Carlin, Richard L. and Duyneveldt, A.J.Van *Magnetic Properties of Transition Metal Compounds*, Inorganic Chemistry Concepts 2, Springer verlag New York Inc., 1977. 6.
Shriver, D.F.; Atkins, P.W. *Inorganic Chemistry*, 1st edition, Oxford university Press,2006. 7. Earnshaw, A. *Introduction to Magnetochemistry*, Academic Press, 1968.
8. Dutta, R.L.; Syanal, A. *Elements of Magneto chemistry*, 2nd edition, Affiliated East West Press, 1993.
9. Drago, Russell S. *Physical Methods for Chemists*, 2nd edition, Saunders College Publishing, 1992.

Course Title: Organic Chemistry-II

L	T	P	Credits	Marks

Paper Code: CHM.509

4	1	0	4	100

Total Lectures: 72

Objective and Learning Outcomes: The objective of this course is that students learn the advanced topics in organic chemistry, and gain depth knowledge in this fundamental branch of Chemistry. A thorough understanding of the content of this course will further prepare students to understand how the computational techniques can be applied to study problems in organic chemistry.

Unit I **14 hrs**

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

Aromaticity: Benzenoid and non-benzenoid compounds – generation and reactions.

Unit II **20 hrs**

Synthetic methodologies: Synthon, Synthetic equivalent, Functional group interconversion (FGI), Functional group addition, Functional group elimination, Criteria for selection of target, Linear and convergent synthesis, Retrosynthetic analysis and synthesis involving chemoselectivity, Regioselectivity, Reversal of Polarity (Umpolung), Synthesis of cyclic molecules, Strategic bond: Criteria for disconnection of strategic bonds, Importance of the order of events in organic synthesis. One group and two group C-X disconnections in 1,2-, 1,3-, 1,4 & 1,5- difunctional compounds, One group C-C disconnections, alcohol and carbonyl compounds, regioselectiviity, alkene synthesis, use of acetylenes and aliphatic nitro compounds in organic synthesis, Two group C-C disconnections, Diels-Alder reaction, 1,3-difunctionalised compounds, Control in carbonyl condensation, 1,5-difunctionalised compounds.

Unit III **16 hrs**

Rearrangements: General mechanistic considerations-nature of migration, migratory aptitude, memory effects, Mechanistic study of the following rearrangements: Pinacol-pinacolone, Wagner-Meerwein, Demjanov, Benzil-Benzillic acid, Favorskii, Arndt-Eister syntheses, Neber, Beckmann, Hofmann Curtius, Schmidt, Baeyer-Villiger, Shapiro reaction, Carroll, Claisen, Cope, Gabriel–Colman, Smiles and Sommelet–Hauser rearrangements.

Selective Name Reactions: Aldol, Perkin, Stobbe, Dieckmann Condensation, Reimer-Tiemann, Reformatsky and Grignard reactions, Diels-Alder reaction, Robinson Annelation, Michael addition, Mannich reaction, Stork-enamine, Sharpless Assymetric Epoxidation, Ene, Barton, Hofmann-Loffler Fretag, Shapiro reaction, Chichibabin Reaction.

Unit IV **22 hrs**

Pericyclic chemistry: Introduction, Main features of pericyclic reactions, Classification of pericyclic reactions. 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. Thermal and photochemical pericyclic reactions.

Electrocyclic reactions: Conrotation and disrotation. Electrocyclic closure and opening in 4n and 4n+2 systems. Woodward-Hoffmann selection rules for electrocyclic reactions. Explanation for the mechanism of electrocyclic reactions by (i) symmetry properties of HOMO of open chain partner (ii) Conservation of orbital symmetry and orbital symmetry correlation diagrams and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Examples of electrocyclic reactions.

Cycloaddition reactions: Suprafacial and antarafacial interactions. $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Cycloreversions. Stereochemical aspects in supra-supra, supra-antara, antara-supra and antara-antara $\pi^2 + \pi^2$ and $\pi^4 + \pi^2$ cycloadditions. Diels-Alder reaction. Woodward-Hoffmann Selection rules for cycloaddition reactions. Explanation for the mechanism of cycloaddition reactions by (i) Conservation of orbital symmetry and orbital symmetry correlation diagrams (ii) Fukui Frontier Molecular Orbital (FMO) theory and (iii) Huckel-Mobius aromatic and antiaromatic transition state method. Endo-exo selectivity in Diels-Alder reaction and its explanation by FMO theory. Examples of cyclo addition reactions.
Sigmatropic reactions: [1,j] and [i,j] shifts. Suprafacial and antarafacial shifts. Selection rules for [lj} shifts. Cope, and Claisen rearrangements. Explanation for the mechanism of sigmatropic reactions by (i) symmetry properties of HOMO (ii) Huckel-Mobius aromatic and antiaromatic transition state method. Introduction to Cheletropic reactions and the explanation of mechanism by FMO theory.

ESSENTIAL BOOKS:

1. Acheson, R.M. (1976). *An introduction to the Chemistry of heterocyclic compounds*, Wiley India Pvt. Ltd., 3rd edition.
2. Ahluwalia, V. K., and Parasar R. K., (2011). *Organic Reaction Mechanism*, Narosa Publishing House (P) Ltd., 4th edition, India.
3. Bansal, R. K., (2012). *Organic Reaction Mechanism*, New Age International (P) Ltd., 4th edition, New Delhi.
4. Bansal, R. K., (2007). *A text book of Organic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
5. Bansal, R.K. (2010). *Hetrocyclic Chemistry*, New Age Inrternational (P) Ltd., 5th edition, New Delhi.
6. Carey B. F. A., Sundberg R.J., (2007). *Advanced Organic Chemistry Part A and Part B, Springer, 5th edition*.
7. Finar, I. L., (2012). *Organic Chemistry Vol. 1*, Pearson Education, 6th edition, UK.
8. Gilchrist, T.L. (1997). *Heterocyclic Chemistry*, Longman, Prentice Hall, 3rd edition, US.
9. Gupta R.R., Kumar M., Gupta V. (2010). *Heterocyclic Chemistry-II Five Membered Heterocycles Vol. 1-3*, Springer Verlag, India.
10. Joule, J.A., Mills, K. (2010). *Heterocyc1ic Chemistry*, Blackwell Publishers, 5th edition, New York.
11. Kalsi, P. S., (2008). *Stereochemistry: Conformation and Mechanism*, New Age International (P) Ltd., 7th edition, India.
12. Kalsi P. S., (2010). *Organic Reactions and Their Mechanisms*, New Age International Publication, 3rd edition, New Delhi.
13. Lowry, T. H., Richardson K. S., (1998). *Mechanism and Theory in Organic Chemistry*, Addison-Wesley Longman Inc., 3rd edition, US.
14. Morrison, R.T., Boyd R.N., (2011). *Organic Chemistry*, Prentice- Hall of India, New Delhi.

15. Mukherjee S. M., Singh S. P., (2009). *Reaction Mechanism in Organic Chemistry*, Macmillan India Ltd., New Delhi.

16. R. Katritzky, (2010). *Handbook of Heterocyclic Chemistr*y Elsevier, 3rd edition, UK.
17. Smith, M. B. (2013). *March's advanced organic chemistry: reactions, mechanisms, and structure*. John Wiley & Sons.
18. Sykes, P., (1997). *A Guide Book to Mechanism in Organic Chemistry*, Prentice Hall, US.
19. Norman, R.O.C.; Coxon, J.M. *Principles of Organic Synthesis*, Blackie Academic & Professional.
20. Warren, S. *Organic Synthesis: The Disconnection Approach*, John Wiley.
21. Cheng, Xue-Min; Corey, E.J. *The Logic of Chemical Synthesis*, John Wiley

Course Title: Physical Chemistry-II
Paper Code: CHM.510

L	T	P	Credits	Marks
4	1	0	4	100

Total Lectures: 72

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

Unit I **20 hrs**

Properties of Gases: Ideal gases, two-parameter equations of state, cubic equation of state for gaseous and liquid states, van der Waals constants in terms of molecular parameters.

Statistical Thermodynamics: The canonical ensemble, distribution law, partition functions for ideal gase: translational, rotational, vibrational, electronic partitions functions. Calculation of Thermodynamic properties in terms of partition functions, Heat capacity, behavior of solids chemical equilibria and equilibrium constant in terms of partition function.

Unit II **16 hrs**

Thermodynamics: The First Law of Thermodynamics, Entropy and the Second Law, Entropy and the Third Law of Thermodynamics. Helmholtz and Gibbs Energies, Phase Equilibria.

Unit III **18 hrs**

Chemical Equilibrium: Gibbs energy is a minimum with respect to the extent to the extent of reaction, Equilibrium constant is a function of temperature, Standard Gibbs energies of formation is used to calculate Equilibrium constant, Direction of reaction spontaneity, Van't Hoff equation, Molecular partition functions and related thermodynamic data.

Unit IV **18 hrs**

Liquid-Liquid Solutions: Partial molar quantities, Gibbs-Duhem equation, Raoult's and Henry's law.

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.

ESSENTIAL BOOKS:

1. Physical Chemistry, G. M. Barrow, TATA MCGRAW-HILL, 2007.
2. Text Book of Physical Chemistry, K. L. Kapoor, MACMILLAN, 2006.
3. Physical Chemistry, A. W. Atkins, W. H. Freeman, and Company, 1997.
4. Physical Chemistry: A Molecular Approach, D. A. McQuarrie, and J. D. Simon,Viva Books, 2011.
5. Kinetics and Mechanism, J. W. Moore, and R. G. Pearson, John Wiley and Sons, 1981.
6. Physical Chemistry, R. J. Silbey, R. A. Alberty, and M. G. Bawendi, Wiley-Interscience Publication, 2013.
7. Physical Chemistry, T. Engel, and P. Reid, Prentice-Hall, 2012.

Course Title: Quantum Chemistry-I
Paper Code: CSC.502

L	T	P	Credits	Marks
4	1	0	4	100

Total Lectures: 72

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

Unit I **20 hrs**

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

Unit II **14 hrs**

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

Unit III **18 hrs**

Symmetry Point Groups: Determination of point group of a molecule, representations, the great orthogonality theorem, character table, construction of character tables for c2v and c3v groups, symmetry adapted atomic basis sets, construction of molecular orbitals. The direct product representation.

Unit IV **20 hrs**

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

Recommended books:

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

Course Title: Physical Chemistry-Practical
Paper Code: CHM.512

L	T	P	Credits	Marks
36		1	2	50

Total Lectures: 36

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

1. Comparison of acid strengths through acid catalyzed methyl acetate hydrolysis.
2. Energy of activation of acid catalyzed hydrolysis of methyl acetate.
3. Determination of partition coefficient of iodine between water and CCl4/equilibrium constant of tri-iodide formation.
4. Conductometric titration of a weak acid with strong base.
5. Conductometric titration of a mixture of weak and strong acids.
6. Potentiometric titration of a strong acid with strong base using quinhydrone electrode.
7. Conductometric titration of KCl with AgNO3.
8. Molecular weight of a non-electrolyte by cryoscopy method.
9. Plateau of GM tube and study of counting statistics.
10. Determination of half-life of a radionuclide.
11. To determine the amount of acetic acid adsorbed at its different concentrations by charcoal and hence verify the Freundlich adsorption isotherm.
12. Determination of dimerisation constant of benzoic acid in benzene solution.

ESSENTIAL BOOKS:

7. An advanced course in practical chemistry, A. K. Nad, B. Mahapatra, and A. Ghoshal, New Central Book Agency (P) Ltd (2000).
8. Physical Chemistry Practical, S. Maity and N. Ghosh, New Central Book Agency (P) Ltd (2012).
9. Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press (2008).

Course Title: Molecular Spectroscopy
Paper Code: CSC.503

L	T	P	Credits	Marks
4	0	0	4	100

Total Lectures: 72

Objective and Learning Outcomes: This is a fundamental course for students who specialize in Physical/Computational Chemistry. The objective of this course is that students learn the basic concepts of molecular spectroscopy from a fundamental point of view. The course will help students understand how spectroscopic transitions come into picture in molecular quantum mechanics.

Unit I **20 hrs**

Basic Principles: Interaction of electromagnetic radiation with matter, time-dependent perturbation theory, harmonic perturbation and transition probabilities, Einstein transition probabilities, selection rules, line-widths and line shapes, Fourier Transforms in spectroscopy. Introduction to Electronic spectra, Born-Oppenheimer approximation, Franck–Condon principle, change of shape on excitation, Jablonski diagram: fluorescence and phosphorescence.

Unit II **20 hrs**

Infra-red and Raman Spectra: Harmonic and anharmonic oscillators, fundamental frequencies, overtones, Morse potential, hot bands, vibration-rotational spectra of HCl, P, Q, R branches, vibrational theories of polyatomic molecules, normal coordinates and their symmetry (CO_2). Molecular polarizability–Raman Effect, pure rotational Raman spectra of linear molecules, vibrational Raman spectra–Raman activity of vibrational, rule of mutual exclusion. Microwave spectra: rigid and non-rigid rotator mode ls, rotational energies of diatomic molecules: moment of inertia and bond length, centrifugal distortion, effect of isotopic substitution.

Unit III **14 hrs**

Magnetic Resonance: Basic Principles, Nuclear Shielding, Chemical Shift, Spin-spin Coupling: AX, AMX, AX_2, AX_3, AX_n, Equivalent Nuclei, Mechanism, Dipolar Coupling.

Unit IV **18 hrs**

Lasers and Laser Spectroscopy: Principles of laser action, laser characteristics, pulsed lasers, laser cavity modes, Q-switching, mode locking, non-linear effects, harmonic generation, examples of lasers: He-Ne, Nd-YAG, dye lasers, femtosecond spectroscopy.

ESSENTIAL BOOKS:

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

Semester III

Objective and Expected Learning Outcomes: The course structure of semester III of this Programme is designed to provide students with courses that build their depth in the field of Computational Chemistry. This semester includes advanced courses in computational chemistry and foundation courses in computer programming. The list of courses to be taught in this semester is provided below.

Course Title: Computational Chemistry
Paper Code: CSC.601

L	T	P	Credits	Marks
4	1	0	4	100

Total Hours: 72

Objective and Learning Outcomes: This is an advanced course for students who specialize in Computational Chemistry. The objective of this course is that students learn the techniques of molecular quantum chemistry and apply them to study chemical and biochemical problems.

Unit I **18 hrs**

Many Electron atoms: Electron correlation, addition of angular momentum, Clebesch-Gordan series, total angular momentum and spin-orbit interaction.

Unit II **18 hrs**

Ab Initio Methods: Review of molecular structure calculations, Hartree-Fock SCF method for molecules, Roothaan-Hartree-Fock method, selection of basis sets.

Unit III **18 hrs**

Electron Correlation and Basis Sets: Configuration Interaction, Multi-Configuration Self-Consistent Field, Multi-Reference Configuration Interaction, Many-Body Perturbation Theory, Coupled Cluster, Basis sets.

Unit IV **18 hrs**

DFT and Force Fields method: Energy as a functional of charge density, Kohn-Sham equations. Molecular mechanics methods, minimization methods, QSAR.

ESSENTIAL BOOKS:

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

Course Title: Research Methodology

L	T	P	Credits	Marks

Paper Code: CSC.602

2	0	0	2	50

Total Lectures: 30

Objective and Learning Outcomes: The course Research Methodology has been framed to introduce basic concepts of Research Methods. The course covers preparation of research plan, reading and understanding of scientific papers, scientific writing, research proposal writing, ethics, plagiarism, etc.

Unit-I **(08)**

Introduction: Meaning and importance of research, Different types and styles of research, Role of serendipity, Critical thinking, Creativity and innovation, Hypothesis formulation and development of research plan, Art of reading and understanding scientific papers, Literature survey, Interpretation of results and discussion.

Unit-II **(07)**

Library: Classification systems, e-Library, Reference management, Web-based literature search engines, Intellectual property rights (IPRs).

Entrepreneurship and Business Development: Importance of entrepreneurship and its relevance in career growth, Types of enterprises and ownership.

Unit-III **(08)**

Scientific and Technical Writing: Role and importance of communication, Effective oral and written communication, Scientific writing, Research paper writing, Technical report writing, Making R and D proposals, Dissertation/Thesis writing, Letter writing and official correspondence, Oral and poster presentation in meetings, Seminars, Group discussions, Use of modern aids; Making technical presentations.

Unit-IV **(07)**

Research and Academic Integrity: Plagiarism, Copyright issues, Ethics in research, and case studies.

Laboratory Safety Issues: Lab, Workshop, Electrical, Health and fire safety, Safe disposal of hazardous materials.

Recommended Books:

1. S. Gupta, *Research Methodology and Statistical techniques* (Deep and Deep Publications (P) Ltd. New Delhi, India) 2005.
2. C. R. Kothari, *Research Methodology* (New Age International, New Delhi, India) 2008.
3. **Web resources:** www.sciencedirect.com for journal references, www.aip.org and www.aps.org for reference styles.
4. **Web resources:** www.nature.com, www.sciencemag.org, www.springer.com, www.pnas.org, www.tandf.co.uk, www.opticsinfobase.org for research updates.

L	T	P	Credits	Marks
0	0	12	6	150

Subject Code: CSC.603
Subject Name: Dissertation

Objective and Learning Outcomes: The objective of this course would be to ensure that the student carries out literature review in his chosen area of research and carries out preliminary research in the topic chosen. In addition, the student shall have to write a 5000 words review of existing scientific literature with simultaneous identification of knowledge gaps that can be addressed through future work.

The evaluation criteria for this course shall be as follows:

Maximum Marks: 150

S.No.	Criteria	Marks
1.	Review of literature	50
2.	Identification of gaps in knowledge	30
3.	References	20
4.	Content of presentation	15
5.	Presentation Skills	15
6.	Handling of queries	20
Total		150

Course Title: Density Functional Theory
Paper Code: CSC.604
Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

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

Unit-I **18 hrs**

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 **18 hrs**

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 **18 hrs**

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 **18 hrs**

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.

Recommended Books:

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: Computer Programming and Scripting
Paper Code: CSC.605
Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

Objective and Learning Outcome: The objective of this course is to introduce students to the art of scientific programming. The theory part of scientific programming language fortran will be taught to students in this course. In addition, the basics of scripting language perl will be introduced to students.

Unit I **18 hrs**

Introduction to Computers and the Fortran language: History and evolution of Fortran language. Basic elements of Fortran: Fortran Character set, structure of Fortran statement, 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 **18 hrs**

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

Unit III **18 hrs**

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 **18 hrs**

Introduction to computer scripting and perl language, Basic elements of perl, perl syntax, executing the perl programs, arrays, lists, hashes, regular expressions, loops and decisions, files and data, running and debugging perl

Book Recommended:

1. Chapman, Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York (2006).
2. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997).
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press (1996).
4. R. L. Schwartz, T. Christiansen, L. Wall, Learning Perl Second Edition, O'Reilly Media (1997).
5. Foy, Mastering Perl First Edition, O'Reilly Media (2007).

Course Title: Computer Programming and Scripting Lab
Paper Code: CSC.606

L	T	P	Credits	Marks
0	0	8	4	100

Objective and Learning Outcome: The objectives of this course is to ensure that the students actually implement the programming concepts learnt in course CSC.605 to develop computer programs. The course structure will thus be strongly aligned to the theory course CSC.605 and will run parallel to it.

Book Recommended:

1. Chapman, Fortran 95/2003 for Scientists and Wngineers, McGraw-Hill International Edition, New York (2006).
2. V. Rajaraman, Computer Programming in Fortran 90 and 95, PHI Learning Pvt. Ltd, New Delhi (1997).
3. W. H. Press, S. A. Teukolsky, W. H. Vetterling, B. P. Flannery, Fortran Numerical Recipes Volume 2 (Fortran 90), Cambridge University Press (1996).
4. R. L. Schwartz, T. Christiansen, L. Wall, Learning Perl Second Edition, O'Reilly Media (1997).
5. Foy, Mastering Perl First Edition, O'Reilly Media (2007).

Course Title: Fundamentals of Molecular Simulations
Paper Code: CSC.607
Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

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

Unit 1 **14 Hours**

Molecular Modeling and Structure - molecular modeling today: overview of problems, tools, and solution analysis, minitutorials with protein and nucleic acid structure as example. Techniques for Conformational Sampling- Monte Carlo, global optimization, etc.

Unit 2 **14 Hours**

Molecular Mechanics: general features, bond stretching, angle bending, improper torsions, out of plane bending, cross terms, non-bonded interactions, Ramachandran diagram point charges, calculation of atomic charges, polarization, van der waals interactions, hydrogen bond interactions, Water models, Force field, all atoms force field and united atom force field.

Unit 3 **14 Hours**

Energy minimization: Steepest descent, conjugate gradient – Derivatives, First order steepest decent and conjugate gradients. Second order derivatives Newton-Raphson, Minima, maxima saddle points and convergence criteria.-non derivatives minimization methods, the simplex, sequential univariative, Newton's equation of motion, equilibrium point, radial distribution function, pair correlation functions, MD methodology, periodic box, Solvent access, Equilibration, cut-offs.

Unit 4 **14 Hours**

Simulation methods : algorithm for time dependence; leapfrog algorithm, Verlet algorithm, Boltzmann velocity, time steps, duration of the MD run, Starting structure, analysis of MD job, uses in drug designing, ligand protein interactions. Various methods of MD, Monte Carlo, systematic and random search methods. Differences between MD and MC, Energy, Pressure, Temperature, Temperature dynamics, simulation softwares. Various methods of MD, Monte Carlo, systematic and random search methods.

Suggested Readings:

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

Course Title: Fundamentals of Molecular Simulations Lab	L	T	P	Credits	Marks
Paper Code: CSC.608	0	0	4	2	50

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

1. Advanced Visualization Software and 3D representations with VMD and Rasmol.
2. Coordinate generations and inter-conversions.
3. Secondary Structure Prediction.
4. Fold Recognition, ab initio method.
5. Homology based comparative protein modeling.
6. Energy minimizations and optimization.
7. Validation of models.
    1. WHATIF
    2. PROSA
    3. PROCHECK
    4. VERIFY 3D
8. Protein Structure Alignment.
9. Modeller
10. Structure based Drug Design
    1. Molecular Docking
    2. De Novo Ligand Design
    3. Virtual Screening
11. Ligand based Drug Design
    1. Pharmacophore Identification
    2. QSAR
12. Molecular Dynamics with Gromacs
13. Binding Site Identification

Suggested Reading

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

Course Title: Modeling Polymeric Materials
Paper Code: CSC.609
Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: This course will introduce the modelling of materials through modern computational tools to analyze materials at nanoscale. It is an initiative to make students familiar with the power of first principles electronic structure theory techniques.

Unit-I **18 hrs**

Materials Modelling through VASP and SIESTA: Basis Sets: plane waves versus numerical atomic orbitals basis sets, Pseudopotentials: ultrasoft versus norm conserving pseudopotentials. Numerical solutions of Kohn-Sham equations, Diagnolization procedure, SCF cycles and mixing scheme, Smearing: Gaussian, Fermi and Methfessel-Paxton smearing.
SIESTA and VASP package to perform: electronic structure calculations, relaxation of atomic positions and unit cell parameters. Structural properties: equilibrium lattice constant, cohesive energy, bulk modulus.

Unit-II **18 hrs**

DFT Calculations for Simple Solids: Crystal structure, Reciprocal lattice, Bonding in crystal, Supercells, Face centered cubic materials, Hexagonal closed packed materials, Crystal structure prediction, Phase transformations, Reciprocal space and k-points**,** Choosing k-points in Brillouin zone, Energy Cutoff, DFT total energies and its relation to various properties, Geometry optimization. Electronic density of states, local density of states and atomic charges, Magnetism.

Unit-III **18 hrs**

DFT Calculations for Surfaces: Periodic boundary conditions and slab model, Calculations of surface energies, Symmetric and asymmetric slab model, Surface relaxation, Surface reconstruction, Adsorbate on surface, Surface Coverage, modelling of one-dimensional systems such as nanotubes, nanoribbons and nanowires, modelling of fullerene-like cages.
DFT Calculations of Vibrational Frequencies: Lattice vibrations and phonons, Isolated Molecules, Vibrations of a collection of atoms, Molecules on surface, Zero-point energies, Phonons and delocalization modes.

Unit-IV **18 hrs**

Calculations beyond Standard DFT: Accuracy of DFT calculations: energy, geometry, vibrational frequencies, Crystal structures and cohesive energies, adsorption energies and bond lengths. DFT+U and DFT+D method for the treatment of electron correlation, Spin-orbit coupling, GW approximation, Excited states properties: dielectric functions and absorption spectra.

Recommended Readings:

1. David S. Sholl and Janice A. Steckel, *Density Functional Theory: A Practical Introduction* (John Wiley and Sons, 2009).
2. June Gunn Lee, *Computational Materials Science: An Introduction*, (CRC Press 2011)
3. C. Kittel, *Introduction to Solid State Physics* (Wiley India (P) Ltd., New Delhi, India) 2007
4. www.vasp.at/index.php/documentation
5. http://departments.icmab.es/leem/siesta/Documentation/Manuals/manuals.htm

Course Title: Computational Chemistry Lab
Paper Code: CSC.610

L	T	P	Credits	Marks
4	0	0	4	100

Course Objective and Learning Outcomes: This course will provide practical experience to the students through use of important Computational Chemistry softwares.

Following experiments will be carried out in the lab.

1. Introduction to Gaussian calculations.
2. Carrying of conformational analysis of small molecules using G09.
3. Vibrational spectra, NMR spectra and TDDFT calculations using G09.
4. Modeling chemical reactions including transition state calculations.
5. 2D potential energy suface generation for two torsion angles.
6. Pseudopotential generation and testing of Si atom.
7. Functional and basis set dependent lattice constant and bulk modulus of Fe solid.
8. Total energy versus cell size and binding energy of H_2 and H_2O molecules.
9. Density of states and electronic band structure of bulk Si.
10. To study the structural and electronic properties of graphene and its nanoribbon.
11. Building macromolecules, extracting crystal structure/NMR coordinates and generating models for MD simulations. RESP charge calculation.
12. Energy minimization during MD simulations- Steepest descent and conjugate gradient methods.
13. Gas phase MD simulations.
14. MD simulations in implicit solvent.
15. MD simulations in Explicit solvents.

References:

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

Course Title: Seminar
Paper Code: CSC.599

L	T	P	Credits	Marks
0	0	8	4	100

Objective and Learning Outcome: The objective of this course would be that students gain in depth knowledge of a chosen topic/research paper, and gain practical presentation skills.

The evaluation criteria for this course shall be as follows:

Maximum Marks: 50

S.No.	Criteria	Marks
1.	Content of presentation	15
2.	Presentation Skills	15
3.	Handling of queries	20
Total		50

Course Title: Dissertation Research
Paper Code: CSC.611
Total Hours: 120

L	T	P	Credits	Marks
0	0	16	8	200

Objective and Learning Outcome: The objective of this course would be to ensure that the student carries research in the topic chosen. The evaluation criteria for this course shall be as follows:

Maximum Marks: 200

S.No.	Criteria	Marks
1.	Continuous assessment by the supervisor	50
2.	First mid-semester presentation (synopsis)	50
3.	Second mid-semester presentation (presubmission)	50
4.	External review and final presentation	50
	Total	200