COURSE STRUCTURE AND SYLLABUS

APPROVED BY THE

BOARD OF STUDIES OF CENTRE FOR COMPUTATIONAL SCIENCES

FOR

MSc Chemistry (Computational Chemistry)

FOR
BATCHES STARTING FROM 2016
Central University of Punjab
Bathinda-151001

Declaration

The syllabus of MSc Chemistry (Computational Chemistry) has been designed
(i) to ensure maximal overlap with the CSIR-NET syllabus.
(ii) 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	10.4%	10-15%
Core Courses	60.5%	50-65%
Elective Courses	29.1%	25-35%

Eligibility Criteria for M. Sc. Chemistry (Computational Chemistry):

Same as the eligibility criteria prescribed for the M. Sc. Chemical Sciences Course of Centre for Chemical Sciences of CUPB.

M. Sc. Chemistry (Computational Chemistry) 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 order to ensure this, wherever possible, computer programming exercises will be given to students based on Chemistry related problems in the courses taught to students in different semesters. 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	**CSC.451**	**Research Methodology**	F	2	-	-	2	25	25	25	25	50
2	**CSC.452**	**Introduction to Computational Sciences**	F	2	-	-	2	25	25	25	25	50
3	**CSC.501**	**Scientific Programming**	C	2	-	-	2	25	25	25	25	100
3	**CHM.502**	**Inorganic Chemistry-1**	C	4	1	-	4	25	25	25	25	100
4	**CHM.503**	**Organic Chemistry-1**	C	4	1	-	4	25	25	25	25	100
5	**CHM.504**	**Physical Chemistry-I**	C	4	1	-	4	25	25	25	25	100
6	**CHM.506**	**Organic Chemistry- Practical**	C	-	-	4	2	-	-	-	-	50
7	**CHM.507**	**Inorganic Chemistry-Practical**	C	-	-	4	2	-	-	-	-	50
8		**Interdisciplinary Elective**	E	2	-	-	2	25	25	25	25	50
Interdisciplinary course offered for other centres:												
8	**CSC.502**	**Chemistry without test tube**	E	2	-	-	2	25	25	25	25	50
		Total		18	3	8	24	-	-	-	-	650

Semester II

S. No.	**Paper Code**	**Course Title**	**Course Type**	**L**	**T**	**P**	**Cr**	**% Weightage**				
								a	**b**	**c**	**d**	
1	**CSC.503**	**Fundamentals of Molecular Simulations**	C	4	1	-	4	25	25	25	25	
2	**CSC.504**	**Molecular Simulations Lab**	C	-	-	4	2	25	25	25	25	
3	**CSC.505**	**Quantum Chemistry-I**	C	4	1	-	4	25	25	25	25	
4	**CHM.512**	**Physical Chemistry - Practical**	C	-	-	4	2	-	-	-	-	
5	**CSC.499**	**Seminar in Computational Sciences**	F	-	-	4	2	-	-	-	-	
6		**Humanities for Science Students**	E	2	-	-	2	25	25	25	25	
Choose any two of these courses:												
6	**CHM.508**	**Inorganic Chemistry-II**	E	4	1	0	4	25	25	25	25	
7	**CHM.509**	**Organic Chemistry-II**	E	4	1		4	25	25	25	25	
8	**CHM.510**	**Physical Chemistry-II**	E	4	1		4	25	25	25	25	
		Total		18	4	12	24	-	-	-	-	

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**	C	4	1	-	4	25	25	25	25	100
2	**CSC.602**	**Computational Chemistry Lab**	C	-	-	4	4	25	25	25	25	50
3	**CSC.551**	**Introduction to Scripting**	F	2	-	-	2	25	25	25	25	50
4	**CSC.552**	**Programming and Scripting Lab**	F	-	-	4	2	-	-	-	-	50
5	**CSC.603**	**Dissertation Research**	C	-	-	8	4	-	-	-	-	100
Choose any one of these courses												
6	**CSC.604**	**Molecular Spectroscopy**	E	4	1	-	4	25	25	25	25	100
7	**CSC.605**	**Introduction to Biochemistry**	E	4	1	-	4	25	25	25	25	100
Choose any one of these courses:												
8	**CSC.606**	**Density Functional Theory**	E	4	1	-	4	25	25	25	25	100
9	**CSC.607**	**Introduction to Quantum Dynamics**	E	4	1	-	4	25	25	25	25	100
10	**CSC.608**	**Statistics for Chemical and Biochemical Applications**	E	4	1	-	4	25	25	25	25	100
	Total			18	3	16	24					600

Semester IV

S. No.	Paper Code	Course Title		L	T	P	Cr	Weightage				e
								a	b	c	d	
1	**CSC.609**	**Dissertation**	C	-	-	32	16	-	-	-	-	400
Select any two of the following courses:												
2	**CSC.610**	**Statistical Thermodynamics and Molecular Reaction Dynamics**	E	4	1	-	4	25	25	25	25	100
3	**CSC.611**	**Introduction to Drug Design and Role of Computers**	E	4	1	-	4	25	25	25	25	100
4	**CSC.612**	**Modeling Polymeric Materials**	E	4	1	-	4	25	25	25	25	100
5	**CSC.613**	**Physical Organic Chemistry**	E	4	1	-	4	25	25	25	25	100
				8	2		20					600

a: <u>Continuous Assessment:</u> Subjective by enlarge
b: <u>Mid-Term Test-1:</u> Based on Objective Type & Subjective Type Test
c: <u>Mid-Term Test-2:</u> Based on Objective Type & Subjective Type Test
d: <u>End-Term Exam (Final):</u> Based on Objective Type Tests
e: Total Marks
L: Lectures **T:** Tutorial **P:** Practical **Cr:** Credits
F: Foundation Course **C:** Core Course **E:** Elective course

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: Research Methodology
Paper Code: CCS.451
Total Lectures: 36

L	T	P	Credits	Marks
2	0	0	2	50

Course 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, laboratory safety issues etc.

Unit-I[1-5] **(09)**

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[1-5] **(09)**

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[1-5] **(09)**

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[1-5] **(09)**

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. R. Kumar, *Research Methodology* (SAGE Publications India Pvt. Ltd., New Delhi, India), 2012.
2. S. Gupta, *Research Methodology and Statistical techniques* (Deep and Deep Publications (P) Ltd. New Delhi, India) 2005.
3. C. R. Kothari, *Research Methodology* (New Age International, New Delhi, India) 2008.
4. Standard /Reputed Journal authors' instructions.
5. **Web resources:** www.sciencedirect.com for journal references, www.aip.org and www.aps.org for reference styles.
6. **Web resources:** www.nature.com, www.sciencemag.org, www.springer.com, www.pnas.org, www.tandf.co.uk, www.opticsinfobase.org for research updates.

Course Title: Introduction to Computational Sciences
Paper Code: CCS.452
Total Lectures: 36

L	T	P	Credits	Marks
2	0	0	2	50

Course Objective and Learning Outcomes: This course has been designed to provide an introductory understanding of the broad filed of Computational Sciences. The course covers various aspects of the field and attempts to provide a bird's eye view of the scientific potential of this growing field.

Unit-I[1,5] **(09)**

Introduction: Overview of Computational Sciences and its applications to Natural Sciences, Nobel Prize winners in Computational Natural Sciences and their contributions to the field, Modelling process and its types, Computational Toolbox- errors and their types, rate of change, fundamental concepts of integral calculus, Importance of Learning Computer Programming in Computational Natural Sciences.

Unit-II[2,5]

Applications of Computational Sciences in Chemistry **(09)**

Computational Quantum Chemistry and its applications, Prediction of Molecular Properties using Computational Chemistry, Overview of Quantum Chemistry Theories and their level of accuracy and hierarchy of computational requirements, Overview of Computer aided drug design and QSAR, Promises of Computational Chemistry

Unit-III[3,5] **(09)**

Applications of Computational Sciences in Physics

Computational Sciences in Molecular Physics, Computational Modeling of materials and prediction of material properties, Overview of Computational Fluid Dynamics and Computational Biophysics, Modeling force and motion, Overview of Cellular Automata Simulations, promises of Computational Physics

Unit IV[4,5]

Applications of Computational Sciences in Life Sciences

(09)

Overview of Computational Biology and bioinformatics, Structural Bioinformatics, Genomic data and its interpretation, Molecular Dynamics Simulations on Biological Systems, Hybrid Computational Methods for Studying Structure, Dynamics and Functions of Large Biological Systems, Promises of Computational Biology.

Recommended Books and References:

1. A. B. Shiflet and G. W. Shiflet. Introduction to Computational Sciences (Overseas Press (India) Pvt. Ltd., New Delhi, India), 2011.
2. F. Jensen. Introduction to Computational Chemistry (Second Edition, Wiley), 2007.
3. J. Hasbun, P. Devries. A First Course in Computational Physics. (Viva Books Pvt. Ltd., New Delhi), 2011.
4. D. W. Mount. Bioinformatics (2nd Edition, Cold Spring harbour Press, New Jersey), 2004.
5. Some examples will be taken from Selected Articles from Standard /Reputed Journals.

Course Title: Scientific Programming
Paper Code: CCS.501
Total Lectures: 36

L	T	P	Credits	Marks
2	0	0	2	50

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

Unit I **(09)**

Introduction to Computers and Fortran and C languages: History and evolution of Fortran and C languages, Basic elements of Fortran and C: Character sets, structure of statements, Structure of a Fortran and C Program, compiling, linking and executing the Fortran and C programs.

Unit II **(09)**

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

Unit III **(09)**

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

Unit IV **(09)**

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 and C.

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

L	T	P	Credits	Marks
2	0	0	2	50

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)**

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)**

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)**

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)**

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: Inorganic Chemistry-I
Paper Code: CHM.503
Total Lectures: 72

L	T	P	Credits	Marks
2	0	0	2	50

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 **(22)**

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)**

Aliphatic nucleophilic subsitution reaction: The SN^2, SN^1, mixed SN^1 and SN^2 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)**

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)**

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., March J., (Latest Ed.) *March's Advanced Organic Chemistry*, John Wiley and Sons, 6th edition, New York.
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.

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

L	T	P	Credits	Marks
2	0	0	2	50

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)**

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)**

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)**

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)**

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: 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

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.

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. Tewari, K.S.; Vishnoi, N.K.; Mehrotra, S.N. A Textbook of Organic Chemistry, 2nd edition, Vikas Publishing House, 1976.
5. Leonard, J.; Lygo, B. Advanced Practical Organic Chemistry, Chapman and Hall, 1995.

Course Title: Inorganic Chemistry Practical
Paper Code: CHM.507
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 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 Ba2+ as its chromate.
2. Estimation of lead as its lead sulfate.
3. Estimation of Nickel (II) as its nickel dimethyl glyoximate.
4. Estimation of Cu2+as cuprousthiocyanate.

Precipitation Titrations

1. AgNO3 standardization by Mohr’s method.
2. Volhard’s method for Cl- determination.
3. Determination of ammonium / potassium thiocyanate.

Oxidation-Reduction Titrations

1. Standardization of KMnO4with sodium oxalate and determination of Ca2+ 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.

Course Title: Chemistry without Test Tube (ID)
Paper Code: CSC.502
Total Hours: 36

L	T	P	Credits	Marks
36	0	0	2	50

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

Unit-I **(09)**

How Science Deals with Complex problems: Level in science, what are molecules made of, interaction between atoms, simplest examples: H_2 and LiH. Thinking in 3D, must we use quantum theory.

Unit-II **(09)**

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 **(09)**

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 **(09)**

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

Recommended 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 some 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, 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 Chemical Sciences of CUPB.

Course Title: Fundamentals of Molecular Simulations
Paper Code: CSC.503
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 careers in academia and industry.

Unit I **(18)**

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 II **(18)**

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 III **(18)**

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 IV **(18)**

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: Molecular Simulations Lab
Paper Code: CSC.504
Total Lecture: 36

L	T	P	Credits	Marks
0	0	4	2	100

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.
    a. WHATIF
    b. PROSA
    c. PROCHECK
    d. VERIFY 3D
8. Protein Structure Alignment.

9. Modeller
10. Structure based Drug Design
    a. Molecular Docking
    b. De Novo Ligand Design
    c. Virtual Screening
11. Ligand based Drug Design
    a. Pharmacophore Identification
    b. 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: Quantum Chemistry-I
Paper Code: CSC.505
Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

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)**

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)**

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

Unit III **(18)**

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)**

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
Total Lectures: 36

L	T	P	Credits	Marks
36		1	2	50

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:

1. An advanced course in practical chemistry, A. K. Nad, B. Mahapatra, and A. Ghoshal, New Central Book Agency (P) Ltd (2000).

2. Physical Chemistry Practical, S. Maity and N. Ghosh, New Central Book Agency (P) Ltd (2012).
3. Collection of Interesting General Chemistry Experiments, A. J. Elias, Universities Press (2008).

Course Title: Seminar
Paper Code: CSC.599

L	T	P	Credits	Marks
0	0	8	4	100

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

The evaluation criteria shall be as follows:

S.No.	Criteria	Marks
1	Content	20
2	Presentation Skills	20
3	Handling of queries	10

Course Title: Inorganic Chemistry-II
Paper Code: CHM.508
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

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)**

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)**

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

Unit III **(15)**

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)**

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
Paper Code: CHM.509
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

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)**

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)**

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)**

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)**

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., March J., (2001). *March's Advanced Organic Chemistry*, John Wiley and Sons, New York.
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. March, Jerry *Advanced Organic Chemistry - Reactions, Mechanism and Structure*, 6th edition, John Wiley, 2007.
21. Warren, S. *Organic Synthesis: The Disconnection Approach*, John Wiley.
22. Cheng, Xue-Min; Corey, E.J. *The Logic of Chemical Synthesis*, John Wiley

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Course Title: Physical Chemistry-II
Paper Code: CHM.510
Total Lectures: 72

L	T	P	Credits	Marks
4	1	0	4	100

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)**

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)**

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)**

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)**

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.

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
Total Hours: 72

L	T	P	Credits	Marks
4	1	0	4	100

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: Computational Chemistry Lab
Paper Code: CSC.602

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: Introduction to Scripting
Paper Code: CSC.551
Total Hours: 36

L	T	P	Credits	Marks
2	1	0	2	50

Objective and Learning Outcomes: The objective of this course is that students learn the basics of computer scripting language perl and python and apply them to study chemical and biochemical problems.

Unit I **(9)**

Introduction to computer scripting and perl language, Basic elements of perl, perl syntax, executing the perl programs, arrays, lists.

Unit II **(9)**

Hashes regular expressions, loops and decisions, files and data, running and debugging perl, advanced concepts in perl

Unit III **(9)**

Introduction to python language, basic elements of python, python syntax, executing the python programs, numbers and operators, variables, using names for data, using built-in types.

Unit IV **(9)**

Python language and the standard library: M aking decisions, functions, classes and objects, files and directories, text processing.

References:

1. Learning Perl, R. L. Schwartz, B. D. Foy and T. Phoenix, O' Reilly 6th Edition (2011).
2. Beginning Python, J. Payne, Wiley India Edition (2010).
3. Perl Basic Practices, D. Conway, O' Reilly 1st Edition (2005).
4. Learning Python, M. Lutz, O' Reilly, Tenth Edition (2012).

Course Title: Programming and Scripting Lab
Paper Code: CSC.552
Total Hours: 72

L	T	P	Credits	Marks
0	1	4	2	50

Course Objective: This course will provide practical experience to the students through applications of Fortran, C, perl and python programming and scripting languages to problems of chemical interest. Thus, this lab course will strongly align with the theory courses CSC.501 (Scientific Programming) and CSC.551 (Introduction to Scripting) to provide practical programming experience to students.

Course Code: CSC.603
Course Name: Dissertation Research

L	T	P	Credits	Marks
0	0	8	4	100

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:

S.No.	Criteria	Marks
1.	Review of literature	30
2.	Identification of gaps in knowledge	10
3.	References	10
4.	Content of presentation	30
5.	Presentation Skills	10
6.	Handling of queries	10
	Total	100

Course Title: Molecular Spectroscopy
Paper Code: CSC.604
Total Lectures: 72

L	T	P	Credits	Marks
4	0	0	4	100

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)**

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)**

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)**

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)**

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).

Course Title: Introduction to Biochemistry

Paper Code: CSC.605

L	T	P	Credits	Marks
4	0	0	4	100

Total Lectures: 72

Objective: This objective of the subject is to ensure that a student understands the structures and purposes of basic components of prokaryotic and eukaryotic cells, especially macromolecules, membranes, and organelles, and how chemical forces and reactions determine their structure and functions in living cells.

Unit I **(18)**

Composition, structure and function of Biomolecules: Carbohydrates, Lipids, Proteins, Nucleic acids and Vitamins. Bioenergetics and metabolism of Carbohydrates, Lipids, Amino Acids and Nucleotides. Stabilizing interactions in biomolecules: Van der Waals, Electrostatic, Hydrogen bonding, Hydrophobic interactions, etc.

Unit II **(18)**

Protein and Nucleic Acid Chemistry: The three dimensional Structure of Proteins Ramachandran plot, Secondary, Tertiary and Quaternary structure, Domains, Motif and Folds. Nucleic acids: A-, B-, Z-DNA, 3D RNA structures, folding and recognition, Stability of protein and Nucleic acid structures.

Unit III **(18)**

Replication, transcription and translation processes: Proposed Mechanisms of reactions and enzymes involved.

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

Unit IV **(18)**

Nucleic Acid Damage and Repair: Introductory level understanding of process of DNA damage and its relation to carcinogenicity, DNA repair- types and enzymes involved.

RNA Structural Informatics: RNA base pairing, RNA molecular recognition, ribozymes.

Suggested Reading:

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. (2008). *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. (2008). *Principles of biochemistry*. CBS Publishers & Distributors. New Delhi, India.

Course Title: Density Functional Theory
Paper Code: CSC.606
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)**

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)**

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)**

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)**

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: Introduction to Quantum Dynamics

Paper Code: CSC.607

L	T	P	Credits	Marks
4	1	0	4	100

Total Lecture: 72

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

Unit I[1-6] **18 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[1-6] **18 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[1-4] **18 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[1-6] **18 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.

Books

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

Course Title: Statistics for Chemical and Biochemical Applications

Paper Code: CSC.608

Total Lecture: 72

L	T	P	Credits	Marks
4	0	0	4	100

Objective: This course will introduce students with fundamentals and applications of statistics to problems of chemical and biochemical interest.

Unit I **(15)**

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

Unit II **(15)**

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

Unit III **(18)**

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

Unit IV **(24)**

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, χ^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.

Suggested Reading:

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

Course Title: Dissertation Research
Paper Code: CSC.609

L	T	P	Credits	Marks
0	0	32	16	400

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: 400

S.No.	Criteria	Marks
1.	Continuous assessment by the supervisor	100
2.	First mid-semester presentation (synopsis)	100
3.	Second mid-semester presentation (presubmission)	100
4.	Final presentation and Defense	100
Total		400

Course Title: Statistical Thermodynamics and Molecular Reaction Dynamics
Paper Code: CSC.610

L	T	P	Credits	Marks
4	1	0	4	100

Total Lecture: 72

Objective: This course will introduce the fundamentals of statistical thermodynamics and molecular reaction dynamics from a physical chemistry perspective.

Unit I **(18)**

Canonical and Grand Canonical Ensembles, Ideal Gas in Canonical and Grand Canonical Ensembles. Partition Function: Rotational, Vibrational and Translational Partition Functions,

Application of Partition Functions to Specific Heat of Solids and Chemical Equilibrium, Real Gases.

Unit II **(18)**

Bose-Einstein Distribution: Bose-Einstein Condensation, Thermodynamic Properties of Ideal BE Gas. Fermi-Dirac Distribution: Degenerate Fermi Gas, Electron in Metals, Magnetic Susceptibility.

Fluctuations: Mean Square Deviation and Fluctuation in Ensembles, Concentration Fluctuation in Quantum Statistics.

Unit III **(18)**

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

Unit IV **(18)**

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.

Book Recommended:

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

Course Title: Introduction to Drug Design and Role of Computers
Paper Code: CSC.611
Total Lecture: 72

L	T	P	Credits	Marks
4	1	0	4	100

Objective and Learning Outcome: The objective of this course is to introduce the students with fundamental aspects of drug design and to illustrate the basic techniques in computer aided drug design.

Unit I **(18)**

Weak Interactions in Drug Molecules; Chirality and drug action; Covalent, ion-dipole, hydrogen bonding, C-H hydrogen bonding, dihydrogen bonding, van der waals interactions and the associated energies, Receptor & biological response, Drug-receptor interactions, receptor theories and drug action: Occupancy theory, rate theory, induced fit theory, macromolecular perturbation theory, activation-aggregation theory. Topological and stereochemical considerations. Theoretical Aspects of Drug Action: Drug distribution, Active transport, Passive transport, The Ferguson Principal Physicochemical Parameters and Pharmacological Activity-Solubility, Partition Coefficient, Surface Activity, pKa, Ionisation, Stereochemical Factors, Bio-isosterism.

Unit II **(18)**

Enzyme Kinetics in Drug Action: Mechanisms of enzyme catalysis, Electrostatic catalysis and desolvation, Covalent catalysis, acid-base catalysis, strain / distortion in enzyme catalysis, Coenzyme catalysis, Theories of enzyme inhibition and inactivation, Enzyme activation of drugs-prodrugs. Drug Metabolism: Metabolic Processes- Phase-I (Oxidation, Reduction & Hydrolysis) and Phase-II (Glucuronide Conjugation, Acetylation, Methylation, Sulphate Conjugation, Conjugation with amino acids and Mercapturic acid formation), Routes of Elimination, Factors Affecting Metabolism–Genetic Factors, Physiological Factors, Pharmaceutical Factors, Drug Interactions.

Unit III **(18)**

Principles of Drug Design and Drug Discovery: History of drug discovery. Drug pharmacokinetics (ADME) and pharmacodynamics. Drug targets and receptor theory. Nature of drug-receptor interactions. Agonists, antagonists and enzyme inhibitors. Natural products as lead structures in drug discovery. Structure pruning technique in lead modification e.g. morphine. Discovery of lead structure from natural hormones or neurotransmitters. Serendipitious discovery of leads e.g. Penicillin and Librium. Existing drugs as leads. Molecular graphics based lead discovery. Principles of design of agonists (e.g. Salbutamol), antagonists e.g. Cimitidine) and enzyme inhibitors (e.g. Captopril). Principles of prodrug design.

Unit IV **(18)**

Lead Modification, SAR studies: Lead modification strategies: Bioisosterism, variation of alkyl substituents, chain homologation and branching, variation of aromatic substituents, extension of structure, ring expansion or contraction, ring variation, variation and position of hetero atoms, ring fusion, simplification of the lead, rigidification of lead. Discovery of oxaminquine, salbutamol, cimitidine and captopril. Structure-Activity Relationship studies in sulfa drugs, benzodiazepines, barbiturates, and taxol analogs. Quantitative Structure Activity Relationship (QSAR) Studies: Introduction to Quantitative Structure Activity Relationship (QSAR) studies. 2-D QSAR, QSAR parameters. 3-D QSAR, CoMFA and CoMSIA. Receptor based 3-D QSAR, molecular docking.

Texts/References

1. Lemke, T. L.; Williams, D. A. Hardcover (2009) Foye's Principles of Medicinal Chemistry. 6th Edition.

2. Ellis, G. P.; West, G. B. Progress in Medicinal Chemistry Series. (1983) Elsevier Science Publication, Volume 20.
3. Lawton, G.; Witty, D. R. (2011) Progress in Medicinal Chemistry Series. Volume 50.
4. Ganellin, C. R.; Roberts S. M., (1993) Medicinal Chemistry: The Role of Organic Chemistry in Drug Research. Publisher: Academics Press Inc.
5. Silverman R. B., (2004) Organic Chemistry of Drug Design and Drug Action, Publisher: Elsevier. 2nd Edition.
6. Lednicer D., Laster A. Mitscher, (1998) The Organic Chemistry of Drug Synthesis (3 Volumes) Publisher: John Wiley & Sons.
7. Lednicer, D. (2008) Strategies for Organic Drug Synthesis and Design Publisher: John Wiley & Sons. 6th Edition.
8. Foye, W. O.; Lemke, T. L.; Williams, D. A. (1995) Principles of Medicinal Chemistry, Publisher: Indian Ed. Waverly, Pvt. Ltd. New Delhi.
9. Kadam, Mahadik, Bothara (2010) Principle of Medicinal Chemistry (Volume I & II), Publisher: Nirali publication
10. Wilson, C. O.; Block, J. H.; Gisvold, O.; Beale, J. M. Wilson and Gisvold's (2003) Textbook of Organic Medicinal and Pharmaceutical Chemistry. Publisher: Lippincott Willaiams & Wikins.
11. Kulkarni, V. M., Bothra, K. G., (2008) Drug Design, Publisher: Nirali Publication. 3rd Edition.

Course Title: Modeling Polymeric Materials
Paper Code: CSC.612
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)**

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)**

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)**

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)**

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

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Course Title: Physical Organic Chemistry

Paper Code: CSC.613

L	T	P	Credits	Marks
4	1	0	4	100

Total Lecture: 72

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

Unit-I[1-6] **(18)**

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

Unit-II[1-6] **(18)**

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[1-6] **(18)**

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[1-6] **(18)**

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.

Recommended Readings:

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