M.Sc. DEGREE COURSE (AUTONOMOUS) IN CHEMISTRY (SEMESTER PATTERN)

CHOICE BASED CREDIT SYSTEM (CBCS)

REGULATIONS - 5

(Effective from the academic year 2017 – 2018 onwards)

SCHOOL OF CHEMISTRY
BHARATHIDASAN UNIVERSITY
TIRUCHIRAPPALLI – 620 024

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1. Name of the Course

Bharathidasan University under choice based credit system (CBCS) is offering a two year M.Sc. Degree Course (Semester Pattern) in Chemistry to be conducted in the School of Chemistry with provision for a research project in the second year.

The term 'credit' is used to describe the quantum of syllabus for various programmes in terms of hours of study. Core courses are a set of compulsory courses required for each programme. Elective courses are suggested by the departmental committee to their students. The minimum credit requirement for two year masters programme in chemistry is 90.

2. Eligibility for Admission

A person who has passed the B.Sc. degree examination with Chemistry as major subject and Mathematics or Physics or Botany or Zoology or any science subject as one of the allied subjects of this University or an examination of any other University accepted by the syndicate of Bharathidasan University as equivalent thereto shall be permitted to appear in the examination of this University, two semesters corresponding to each year of study, and qualify for the M.Sc. Degree in Chemistry. A candidate seeking admission to the course shall not be more than 25 years of age on 1st July of the year of admission.

3. Duration of the Course

The course for the degree of Master of Science in Chemistry shall consist of four semesters, two in the first year and two in the second year.

4. Examination

For the purpose of these regulations, the academic year shall be divided into two semesters, the first being from 1st July to 30th November and the second from 1st December to 30th April. The University examinations (end semester examinations) in

the first/third semester shall be conducted in November and the examinations (end semester examinations) in the second/fourth semester in April.

A candidate who does not pass the examination in any subject or subjects of the first, second and third semesters will be permitted to reappear in such subject(s) to be held in April and November in the subsequent semester/year.

A candidate should get registered for the first semester examination. He/She shall register for subsequent semester examinations only after registering for the previous semester examinations.

5. Course Features

The programme consists of core courses (CC) and elective courses (EC) distributed among the four semester periods. The core courses include theory, practical and project work (seminar, project report and viva voce).

6. Course Structure: See ANNEXURE I and Part A

7. Courses offered to students of other department: See Part B

8. CHE544CC Project Work

The project guide for the project work will be chosen by the students based on the academic ranking in the first semester at the end of the second semester and students will carry out the project work during both the third and fourth semesters (i.e., during the second year). The project report shall be submitted to the School of Chemistry on a date notified before the end of fourth semester. Uniformity in writing and presentation of matter in the report shall have to be maintained for proper evaluation. e.g., references are to be indicated by superscripts in the body and indexed in detail at the end. The project shall be evaluated by two examiners nominated by the Head of the Department, one of whom shall be the project guide.

The project work will be evaluated by the guide and external examiner separately. Then there will be a viva-voce conducted jointly by the guide and external examiner. Based on the evaluation of the dissertation and the performance of the candidate in the viva voce, the marks will be awarded as indicated below:

For evaluation of project work,

(i)	Project seminar (internal)	=	25 marks
(ii)	By the Guide	=	25 marks
(iii)	By the External Examiner	=	25 marks
(iv)	Viva voce by Guide and External examiner	=	25 marks
	Total	=	**100 marks**

If the student gets a total mark of less than 50 then the project work will be treated as rejected and the student will be declared as failed in the course. The failed student can resubmit the project report on a date notified at the end of November or April in the

subsequent semester/year. The resubmission is permitted up to a maximum of three times.

9. Condonation

Students must have 75% of attendance in each semester to appear for the examination. Students who have attendance between 65% and 74% shall apply for condonation in the prescribed form with the prescribed fee. Students who have attendance between 50% and 64% shall apply for condonation in prescribed form with the prescribed fee along with the Medical Certificate.

Students who have attendance below 50% are not eligible to appear for the examination. They shall re-do the semester(s) after completion of the Programme (i.e. 2 years).

10. Question Paper Pattern

Section A : 10 Questions x 2 Marks = 20 Marks
(Two questions from each unit)
Section B : 5 Questions x 4 Marks = 20 Marks
(Internal Choice and one set of questions from each unit)
Section C : 5 Questions x 7 Marks = 35 Marks
(Internal Choice and one set of questions from each unit)

11. Continuous Internal Assessment (CIA)

a) The marks assigned for the continuous internal assessment in theory shall be based on:

i. Regularity in attendance
ii. Performance in midterm and model tests conducted
iii. Submission of assignments
iv. Participation in seminars

b) The marks assigned for the continuous internal assessment in practical shall be based on:

i. Regularity in attendance
ii. The number of exercises completed satisfactorily
iii. The results, skill and tidiness of work
iv. Maintenance of laboratory observation note books and submission of laboratory record note books

12. Practical Examinations

During the practical examination in each subject at the end of first and second semesters, each student should take a viva-voce examination (5 marks) when the

examiners shall test the candidate's general understanding of theoretical concepts relating to the experiments done.

13. Panel of Examiners

The theory examination shall be evaluated by external examiner (except in case of interdisciplinary papers) and the practical examination and project work shall be assessed by two examiners – one external and the other internal.

14. Passing Minimum

A student is declared as passed in a subject when he secures minimum of 50% inclusive of external and internal assessments and a minimum of 40% component of the final external exam marks (30 out of 75).

15. Grading of the Course and Classification of Successful Candidates: See **ANNEXURE II**

16. Statement of Marks and Grades

All the statements of course credit and grades for all the semester examinations and provisional degree certificate will be signed and issued by the Controller of Examinations. For details on calculation of grading see annexure –II.

17. Conferment of the Degree

A candidate shall be eligible for the conferment of the master Degree in chemistry only after he/she has earned a minimum of 90 credits.

18. Ranking

A candidate who passes the whole examination in first class within the prescribed period of duration of the course in the first appearance in all the examinations and scores the highest CGPA is alone eligible for ranking. Rank certificate will be issued for the first two positions only.

19. Span Period of Course

The candidates who are admitted on or after 2015-2016 onwards be allowed to complete the PG programmes within two years from completion of programme. In exceptional circumstance a further extension of one more year may be granted. The exceptional circumstances be spelt out clearly by the relevant statutory body concerned of the University. During the extended period the student shall be considered as a private candidate and also not be eligible for ranking. Further, the private candidates will be permitted to appear only for two chances to complete their respective degree course.

20. Transitory Provision

Candidates who have joined the course in the academic years 2012–2013, 2013–2014, 2014-2015, 2015-2016 and 2016–2017 will be permitted to appear for examination under the respective old regulations for a period up to and inclusive of the examination in April 2020. Thereafter, they will be permitted to appear for the examination only under the regulations in force at that time.

21. Revision of Regulations and Curriculum

The Department of Chemistry may from time to time amend and change the regulations and the curriculum as and when necessary.

ANNEXURE - I

6. Course Structure

Semester	COURSE Code No	Title of the Course Paper	Credits	CIA	ESE	Total
First Semester	CHE511CC	Organic Chemistry – I	5	25	75	100
	CHE512CC	Inorganic Chemistry – I (Main Group and Coordination Chemistry)	5	25	75	100
	CHE513CC	Physical Chemistry – I	5	25	75	100
	CHE514CP	Organic Chemistry Practical – I	3	25	75	100
	CHE515CP	Inorganic Chemistry Practical -1	3	25	75	100
	CHE516CP	Physical Chemistry Practical– I	3	25	75	100
Second Semester	CHE521CC	Organic Chemistry – II	5	25	75	100
	CHE522CC	Inorganic Chemistry – II (Bio-Inorganic and Organometallic Chemistry)	5	25	75	100
	CHE523CC	Physical Chemistry – II	5	25	75	100
	CHE524CP	Organic Chemistry Practical – II	3	25	75	100
	CHE525CP	Inorganic Chemistry Practical – II	3	25	75	100
	CHE526CP	Physical Chemistry Practical –II	3	25	75	100
Third Semester	CHE531EC	Organic Chemistry-III	5	25	75	100
	CHE532CC	Inorganic Chemistry – III (Physical Methods in Inorganic Chemistry)	5	25	75	100
	CHE533CC	Physical Chemistry – III	5	25	75	100
	CHE534EC	Advanced Topics in Chemistry -III	5	25	75	100
Fourth Semester	CHE541CC	Organic Chemistry – IV	5	25	75	100
	CHE542EC	Inorganic Chemistry – IV (Selected Topics in Inorganic Chemistry)	5	25	75	100
	CHE543EC	Physical Chemistry-IV	5	25	75	100
	CHE544CC	Project Work	7	25	75	100
Total Credits			90			

CIA : Continuous Internal Assessment, **ESE :** End Semester Examination, **CC:** Core Course, **EC:** Elective Course

INTERDEPARTMENTAL COURSES FOR OTHER DEPARTMENTS

Sl. No.	Course Code	Course Title	Credit	CIA Marks	ESE Marks	Total Marks
1	CHE526-1EC	Selected Topics In Chemistry-I	4	25	75	100
2	CHE526-2EC	Concepts and Models in Chemistry	4	25	75	100
3	CHE535-1EC	Selected Topics In Chemistry-II	4	25	75	100
4	CHE535-2EC	General Chemistry	4	25	75	100

VALUE ADD ON COURSES

Sl. No.	Course Code	Course Title	Credit	CIA Marks	ESE Marks	Total Marks
1	CHE511AC	Medicinal Chemistry	2	40	60	100
2	CHE521AC	Environmental Chemistry	2	40	60	100
3	CHE531AC	Materials Chemistry	2	40	60	100
4	CHE541AC	Polymer Chemistry	2	40	60	100

PROGRAMME OUTCOMES

- The chemistry faculty will strive to maintain a quality program in which faculty are knowledgeable in the subject matter being taught, including current research areas, and are enthusiastic about working with students at the undergraduate and graduate levels.
- The chemistry faculty will continue to review and revise the curriculum to ensure that it is rigorous, logically sequenced, and reflective of the current state of the field.
- Students graduating with a Master degree in chemistry should be proficient in the advance level of chemistry.
- Students graduating with a Master degree in chemistry will be prepared for entry into research program, or the job market.
- Students graduating with a chemistry certification will have a chemistry background that will allow them to become effective Scientist or teachers in the higher education.

PROGRAMME SPECIFIC OUTCOMES

- Gains complete knowledge about all fundamental aspects of all branches of chemistry
- Understands the basic concepts behind complex chemical structures, reagents in organic syntheses, reactive intermediates, important organic reactions and its mechanisms, naming reactions, molecular rearrangements, stereochemistry, instrumental method of chemical analysis and natural products etc.
- Identify the importance of various elements present in the periodic table, coordination chemistry and structure of molecules, properties of compounds, structural determination of complexes using theories and instruments, complex metal drugs and catalysts, role of metal ions in biological processes and organometallic chemistry
- Gathers attention about the physical aspects of atomic structure, quantum chemistry, thermodynamics, reaction pathways with respect to time, various energy transformations, significance of electrochemistry, molecular spectroscopy, role of catalysts in reactions, polymer chemistry, materials chemistry and bio-physical chemistry.
- Learns about the potential uses of analytical industrial chemistry, medicinal chemistry, and environment oriented chemistry.
- Apply the various analytical techniques like IR, mass, NMR, NQR, EPR, XRD to structural characterization of unknown compounds.
- Carry out experiments in the area of organic analysis, estimation, separation, derivative process, inorganic semi micro analysis, preparation, conductometric and potentiometric analysis
- Obtain knowledge in Spectral, Analytical, Qualitative & Quantitative techniques and contribute new scientific insights or innovative applications of chemical research to the next generation.

ANNEXURE – II

15. Grading of the Course and Classification of Successful Candidates

Once the marks of the CIA and the end-semester examination for each of the courses are available, they will be added. The marks thus obtained, will then be graded as per the scheme provided in Table 1.

Table 1 Grading of the Courses Final Result

MARKS RANGE	GRADE POINT	GRADE	DESCRIPTION
90-100	10	O	Outstanding
80-89	9	A+	Excellent
70-79	8	A	Very good
70-69	7	B+	Good
50-59	6	B	Average
Below 50	5	N.A	Re-appearance
-	0	AAA	Absent

From the second semester onwards the total performance within a semester and the continuous performance starting from the first semester are indicated by **Semester Grade Point Average (GPA)** and **Cumulative Grade Point Average (CGPA),** respectively. **CGPA**= Average GPA of all the Courses starting from the first semester to the current semester. These two are calculated by the following formulae:

Classification:

CGPA	9 and above and should have passed all Papers in the first appearance	I	Class with Distinction
CGPA	7 and above but less than 9	I	Class
CGPA	5 and above not less than	II	Class

Note : The above classification shall be given for

1. Over all performance including non-major electives and skill based courses
2. For performance in the Part I, II, III and IV individually.

Formulae for GPA and CGPA

$$GPA_j = \frac{\sum_{i=1}^{n} C_i G_i}{\sum_{i=1}^{n} C_i} \qquad \text{Weighed average Marks} = \frac{\sum_{i=1}^{n} (C_j M_j)}{\sum_{i=1}^{n} C_j}$$

Where C_i : Credit assigned to the i-th course, 'G_i' is the Grade Point obtained by the student for the Course i. $\sum$: summation sign. M' is the Marks obtained for the course i and 'n' is the number of Courses **passed** in that semester. The classification of final results shall be based on the CGPA, as indicated in Table 1. Credit based weighted Mark System is to be adopted for individual semesters and cumulative semesters in the column 'Marks Secured' (for 100).

Course Details

PART A

SEMESTER-I **HOURS/WEEK: 6**
CHE511CC **CREDITS: 5**

ORGANIC CHEMISTRY - I

OBJECTIVES

- To learn nomenclature of organic compounds
- To learn stereochemistry of organic compounds
- To understand methods of determining reaction mechanisms and reactive intermediates
- To understand the basic concepts of aromaticity, structure and reactivity
- To study the concepts of molecular rearrangement and their mechanism

UNIT I

1. Nomenclature and Methods of Determining Reaction Mechanisms

Nomenclature of alicyclic, bicyclic and tricyclic compounds (basic skeletal structures only, with or without one substituent) – Types of mechanism and reaction - Characteristics of nucleophilic, electrophilic and free radical reactions – Thermodynamic and kinetic requirements of a reaction – Kinetic and Thermodynamic Control of reactions- Hammond's postulate – Energy profile diagrams – Intermediate versus transition state – Analysis of product and intermediate – Study of Catalysis - Isotopic labeling – Stereochemical studies – Crossover experiments – Kinetic methods– Isotopic and substituent effects.

UNIT II

2. Stereochemistry and Conformation Analysis

Stereoisomerism – Chirality and symmetry – Enantiomers and diastereomers – Fischer, Sawhorse, Newman and chain representations and their interconversions – D-L, erythro-threo, R-S, E-Z nomenclature – Chirality in molecules with non-carbon stereocenters (N, S and P) – Chirality in molecules devoid of stereocenters: allenes, spiranes, biphenyls, helicenes and cyclophanes – Methods of determining configuration – Separation of enantiomeric mixtures (kinetic, enzymatic, chromatographic resolutions) – Prochirality and topicity – Stereospecific and stereoselective reactions – Conformational analysis of cyclopentane, cyclohexane, cyclohexene and fused (decalin) and bridged (norbornane type) ring systems – Anomeric effect in cyclic compounds.

Unit III

3. Aromaticity

Compounds with aromatic sextets: Five-, six-, seven- and eight-membered rings and other systems – Huckel's theory of aromaticity – Electron occupancy in MO's – NMR concept of aromaticity and antiaromaticity - Systems with $(4n + 2)\pi$ electrons and $4n\pi$ electrons – Alternant and non-alternant hydrocarbons – Aromatic systems with 2,4,8 and 10 electrons – Systems of more than 10 electrons (Annulenes) – Mobius aromaticity – Aromaticity in sydnones and fullerenes – Concept of homoaromaticity – Heteraromatic molecules.

UNIT IV

4. Reactive Intermediates

Structure, stability, generation and reactivity of cabocations – Bridged (non-classical) cabocations. Structure, stability, generation and reactivity of carbanions – Acidity of hydrocarbons. Structure, reactivity and generation of carbenes – Reactions of carbenes: Cycloaddition including Simmons-Smith reaction – Insertion to C-H and X-H bonds – Rearrangements – Reactions with nuclophiles.

Structure, reactivity and generation of nitrenes – Reactions of Nitrenes: Cycloaddition, Insertion and Rearrangements.

Structure, reactivity and generation of Benzynes – Reactions of Benzynes: Nucleophilic addition, Cycloaddition.

Generation and characterization of Radicals – Radical ions – Reactions of Radicals: Addition of HX, Halomethanes, Reactions involving Bu_3SnH, Substitution of Halides, McMurry and Eglinton Reactions.

UNIT V

5. Molecular Rearrangements

Carbocation rearrangements – Migratory aptitude and memory effect – 1,2-Shifts, Wagner-Meerwein – Rearrangements involving electron–deficient species: Wolff – Lossen – Schmidt – Baeyer-Villiger – Stevens – Favorski – Sommelet-Hauser – Demyanov – Pummerer – Von-Richter – Dienone-phenol rearrangements.

UNIT VI (Not for final examination)

6. Structure and reactivity

Chemical bonding and basis of reactivity- Chemical bond, delocalization, conjugation, resonance, hyperconjugation, tautomerism, inductive effects, MOT and VBT approach - Bonding other than covalent bonding: Ionic, hydrogen bond, inclusion compounds, rotaxanes, catenanes, cyclodextrins, cryptands, fullerenes, crown ethers - Acidity and basicity: various structural effects, hard and soft acid and base concept.

Text and Reference Books

1. J. March, M.B. Smith, Advanced Organic Chemistry: Reactions, Mechanisms and Structure; 6th Ed., Wiley, New York, 2007.
2. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry; Parts A & B, 5th Ed., Springer, Germany, 2007.
3. T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, Addison-Wesley, 1998.

4. D. Nasipuri, Stereochemistry of Organic Compounds-Principles and Applications, 4th Ed., New Academic Science Limited, 2012.
5. E.L. Eliel, S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley, 2008.
6. P.S. Kalsi, Stereochemistry, New Age International, 2005.
7. I.L. Finar, Organic Chemistry, Vol.II, 5th Ed., Pearson Education, 2013.
8. R.K. Bansal, Organic Reaction Mechanisms, New Academic Science, 2012.
9. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th Ed., Pearson, 1992.
10. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., Oxford University Press; 2012.
11. C.J. Moody and G.H. Whitham, Reactive Intermediates, Oxford University Press; 1992.
12. H.O. House, Modern Synthetic Reactions, 2nd Ed., W. A. Benjamin, New York, 1998.
13. Name reactions and rearrangements in Organic Chemistry, Ratan Kar, Books and Allied (P) Ltd, Kokata, India, 2017.

LEARNING OUTCOMES

After completion of this course, students will be able to understand about

- Reactive intermediates and its properties
- Nomenclature and methods of determining reaction mechanisms
- Aromaticity of organic compounds and its applications
- Understand the various types of aromaticity
- Applications of Huckel's theory to various aromatic compounds and predict their stability
- Stereochemistry and conformation analysis of organic molecules
- Predict the stereochemistry of various organic compounds
- The concepts of molecular rearrangements and their mechanisms

SEMESTER-I **HOURS/WEEK: 6**
CHE512 CC **CREDITS: 5**

Inorganic Chemistry - I

(Main Group and Coordination Chemistry)

OBJECTIVES

- To learn the theories of bonding in small molecules and ionic model
- To understand the basic concepts of main group elements
- To study the principles, bonding concepts and reaction mechanism of coordination compounds

UNIT I

1. Main Group Chemistry

Hydrogen and its compounds: Hydrides: Classification, electron deficient, electron precise and electron rich hydrides. PH_3 , SbH_3 , AsH_3 , Selenides, Tellurides - Alkali and alkaline earth metals: Solutions in non-aqueous Media, Application of crown ethers in extraction of alkali and alkaline earth metals - Organometallic Compounds of Li, Mg, Be, Ca, Na: Classification, Synthesis, Properties, Uses and Structure - Carbon Group: Allotropes of Carbon, C60 and compounds (fullerenes) - Intercalation compounds of Graphite, Carbon nanotubes, synthesis, properties, structure-single walled, multi walled, applications - Organometallic compounds of Si, Sn, Pb, Ga, As, Sb, Bi. Structures, synthesis, Reactions - Oxygen Group: Metal Selenides and Tellurides, oxyacids, and oxoanions of sulphur & nitrogen - Ring, Cage and Cluster compounds of p-block elements. Silicates, including Zeolites - Halogen Group: Interhalogens, pseudohalagen, Synthesis, Properties and Applications, Structure, Oxyacids and Oxoanions of Halogens, Bonding

UNIT II

2. Main Group Chemistry – Rings, Cages and Clusters.

Chemistry of boron – Classification, diborane structure and bonding, higher boranes, carboranes, borazines and boron nitrides.

Chemistry of silicon – Classification of silicates, Silicones-siloxanes, silanes, higher silanes, silicon nitrides.

P-N compounds-linear and cyclic phosphazenes, S-N compounds – structure and bonding of S_4N_4, polythiazyl $(SN)_x$ compounds

Cluster compounds – Bi, tri, tetra and hexanuclear clusters(Metal halides and oxides only), Wade's rule, polyatomic Zintl anions and cations.

UNIT III

3. Coordination Chemistry: Principles

Lewis acids and Lewis bases in coordination chemistry, detection of complex formation in solution; Stability constants, stepwise and over-all formation constants, methods of determining the formation constants – spectrophotometric method, Job's method and potentiometric method. Factors affecting stability (properties of both metal ions and

ligands, Irwing-William series) – statistical and chelate effects –Class (a) and class (b) acids and bases- HSAB Principle and its applications.

UNIT IV

4. Coordination Chemistry: Theories of Metal-Ligand Bond

VB theory, Crystal field theory and their limitations; splitting of d-orbitals under octahedral, square planar, square pyramidal, trigonal bipyramidal and tetrahedral field, factors affecting crystal field splitting; CFSE for d^1 to d^{10} system, low and high spin complexes, applications of CFSE; spectrochemical series – Jahn-Teller distortion; Ligand field theory, MO theory-sigma bonding in octahedral, square planar and tetrahedral complexes – pi bonding in octahedral complexes.

UNIT V

5. Coordination Chemistry: Reaction Mechanism

Labile and inert complexes, kinetics of octahedral substitution, reaction profile of dissociative and associative mechanism, acid hydrolysis, factors affecting acid hydrolysis, base hydrolysis, conjugate base mechanism, evidences of conjugate mechanism, anation reaction reactions without metal ligand bond cleavage.
Substitution reactions in square planar complexes- mechanism, trans effect-theories and applications, Interconversion between stereoisomers; Redox reactions
Redox Reactions-Electron transfer reactions (complementary and non-complementary types, inner sphere and outer sphere processes), Marcus-Hush Theory.

UNIT VI (Not for final examination)

6. Bonding in Small Molecules

Valence Bond (VBT) and Molecular Orbital (MO) Theories - Application to small molecules such as $BeCl_2$, BCl_3 and CCl_4, SF_4, ClF_3, BrF_3 , BrF_5 , IF_5, IF_7 etc – Bonding in Noble gas compounds – $XeCl_2$, XeF_4, $XeOF_4$, XeF_6.

7. Ionic Model

Lattice energy – Born-Haber Cycle and its application-Born-Lande equation- Madelung Constant- Kapustinski equation. Structure of some ionic crystals: NaCl, CsCl, Rutile, Wurtzite, Fluorite

Text Books

1. M.C. Day and J. Selbin, *Theoretical Inorganic Chemistry*, 2nd Ed., East West Press, 1985.
2. F.A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann,*Advanced Inorganic Chemistry;*6thEd., A Wiley-Interscience Publication, John–Wiley & Sons, USA, 1999.
3. J.E. Huheey, E. A. Keiter, and R.L. Keiter, *Inorganic Chemistry; Principles of Structure and Reactivity*4thEd., Harper & Row publisher, Singapore, 2006.

4. S.F.A. Kettle, *Physical Inorganic Chemistry – A Coordination Chemistry Approach*, Oxford University Press, 1998.
5. D.E. Douglas, D.H. McDaniel, J.J. Alexander, *Concepts and Models in Inorganic Chemistry*, 3rd Ed.1994.
6. J.D. Lee, *Concise Inorganic Chemistry*, 5th Ed, Wiley, 2008.
7. D.F. Shriver, P.W. Atkins, *Inorganic Chemistry*, 5th Ed,2009.
8. A.G. Sharpe, *Inorganic Chemistry*, Pearson Prentice Hall, 3rd Ed. 2008.
9. A. K. Das *Fundamental Concepts of Inorganic Chemistry*, Vol 1-7, CBS publishers, 2nd Ed. 2010.
10. B. Sivashankar, *Inorganic Chemistry*, Pearson (India), 1st Edition, 2013.
11. W. U. Malik, G. D. Tuli, R. D. Madan *Selected Topics in Inorganic Chemistry* S Chand & Company New Delhi, 8th Revised Ed. 2014.
12. Inorganic Chemistry: Shriver & Atkins (4th edition 2003, Oxford)

Reference Books

1. F. Basolo, R.G. Pearson, Mechanism of Inorganic Reactions, 2nd Ed., John Wiley, 1967.
2. L. Pauling, The Nature of the Chemical Bond, 3rd Ed., Cornell University Press, 1960.

LEARNING OUTCOMES

By the end of this course will be able to

- Understand the chemistry of main group elements
- Demonstrate the models and types of ionic crystals
- Know the structure and bonding in molecules / ions and predict their structure
- Learn the principles and applications of coordination chemistry
- Describe the stability of metal complexes by the use of different parameters
- Demonstrate various theories explain the structure and properties of coordination compounds
- Learn the principles of different types of inorganic reactions mechanisms
- Understand different types of electron transfer reactions

SEMESTER-I **HOURS /WEEK: 6**
CHE513CC **CREDITS: 5**

PHYSICAL CHEMISTRY – I

OBJECTIVES

- To understand the basic concepts and applications of group theory, surface chemistry, catalysis and thermodynamics
- To learn the theories of kinetics

UNIT I

1. Group theory - Concepts

Elements of group theory – definition – group multiplication tables – conjugate classes, conjugate and normal subgroups – symmetry elements and operations – point groups – assignment of point groups to molecules - Matrix representation of geometric transformation and point groups – reducible and irreducible representations– properties of irreducible representation – construction of character tables – bases for irreducible representation – direct product – symmetry adapted linear combinations – projection operators.

UNIT II

2. Group Theory: Applications

Symmetry aspects of molecular orbital theory – planar π-systems – symmetry factoring of Huckel determinants – solving it for energy and MOs for ethylene– sigma bonding in AX_n molecules – Formation of hybrid orbitals in molecules like tetrahedral, square planner, trigonal planar, linear, trigonalbipyramidal systems– Selection rules for electronic transition in carbonyl chromophore – vibrational spectra – symmetry types of normal molecules – symmetry coordinates – selection rules for fundamental vibrational transition - IR and Raman activity of fundamentals in CO_2, H_2O, N_2F_2, - the rule of mutual exclusion and Fermi resonance.

UNIT III

3. Reaction Kinetics

Basic kinetic concepts - Theories of reaction rates-collision theory - Transition State theory and its applications – Effect of solvent, ionic strength and pressure on reaction rates - Arrhenius equation – Various theories of unimolecular reactions (Lindemann, Hinshel wood, RRK, RRKM and Slater treatments)

Enzyme catalysis: Michaelis–Menton kinetics for single substrate reactions. Introduction to LFER.Significance of reaction coordinate and potential energy surfaces.

Fast Reaction Kinetics: Relaxation methods, Stopped flow method, Laser Flash Photolysis. Molecular beam studies.

UNIT IV

4. Surface chemistry and Heterogenous catalysis

Surface Phenomena: Gibbs adsorption isotherm – solid- liquid interfaces – contact angle and wetting – solid-gas interface – physisorption and chemisorption – Langmuir, BET

isotherms – surface area determination. Kinetics of surface reactions involving adsorbed species – Langmuir-Hinshelwood mechanism, Langmuir – Rideal mechanism – Rideal –Eley mechanism. Basic aspects of semiconductor catalysis and applications.

UNIT V

5. Thermodynamics-I

Third law-thermodynamics-Need for it-Nernst heat theorem and other forms of stating the third law.Thermodynamic quantities at absolute zero – Apparent exceptions to the third law.

Thermodynamics of systems of variable composition – partial molar properties – chemical potential – relationship between partial molar quantities – Gibbs Duhem equation and its applications (the experimental determination of partial molar properties not included).

Thermodynamic properties of real gases – fugacity concept – calculation of fugacity of real gas – Activity and activity coefficient – concept – definition – standard states and experimental determinations of activity and activity coefficient of electrolytes.

UNIT VI (Not for final examination)

6. Thermodynamics-II

The second law of thermodynamics – Entropy - Activity and Fugacity- determination of fugacity, Nernst equation, Chemical equilibrium - temperature dependence, Vant-Hoff equation, Non-equilibrium thermodynamics - postulates and methodology - Phase equilibrium-Application to three component system - Molecular Thermodynamics - Molecular energy levels, Boltzman distribution law, partition functions and ensembles, translational, rotational and vibrational partition functions of diatomic molecules, Obtaining energy, heat capacity, entropy, free energy, equilibrium constants from partition functions, equipartition of energy.

Text Books

1. F.A. Cotton, Chemical Applications of Group Theory, 3rd Ed., John Wiley & Sons, 2004
2. V.Ramakrishnan and M.S.Gopinathan, Group Theory in Chemistry, Vishal, 1988.
3. H. Metiu, Physical Chemistry, Kinetics Taylor & Francis, 2006
4. K.J. Laidler, Chemical Kinetics, 3rd Ed., Pearson Education, 2004.
5. S. Glasstone, Text Book of Physical Chemistry, Macmillan, 1969.
6. Bond, Heterogeneous Catalysis – Principles and Applications, Clarendon, 1974.
7. J. Rajaram, J.C. Kuriacose, Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible,3rd Ed., ShobhanLalNagin, 2013.
8. G.W.Castellan, Physical Chemistry, Narosa, 2004.
9. I.M. Klotz, P.M. Rosenberg, Chemical Thermodynamics: Basic Concepts and Methods, 7th Ed., John Wiles & Sons, 2008.

Reference Books

1. R.L. Carter, Molecular Symmetry and Group Theory John Wiley, 1998.
2. R.L. Flurry, Jr, Symmetry Groups – Prentice Hall, New Jersy 1980.
3. B.E. Douglas and C.A. Hollingsworth, Symmetry in Bonding and Spectra – An Introduction, Academic Press, 1985.

4. S.F.A. Kettle, Symmetry and Structure, John Wiley & Sons, 1985
5. A.A. Frost, R.G.Pearson, Kinetics and Mechanism, John Wiley & Sons, 1953
6. D.A. McQuarrie, J.D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt Ltd, 2003.
7. J.N. Gurtu, A. Gurthu, Advanced Physical Chemistry, PragathiPrakashan, 2006.
8. R.S. Berry, S.A. Rice, J. Ross, Physical Chemistry, 2nd Ed, Oxford Univ. Press, 2000.
9. J. I. Steinfeld, J.S.Francisco, W.L. Hase, Chemical Kinetics and Dynamics, 2nd Ed, Prentice Hall, 1999.
10. K.S. Gupta, Chemical Kinetics and Reaction Mechanism, RBSA Publishers, 1992.
11. R. K. Dave, Chemical Kinetics, Campus Books, 2000.
12. A.W. Adamson, Physical Chemistry of Surfaces, 4th Ed., John Wiley, 1982.
13. B.M.W. Trapnell, Chemisorption, Academic Press, 1955.
14. D.A. McQuarrie, J.D. Simon, Molecular Thermodynamics, University Science Books, 1999
15. Glasstone, Thermodynamics for Chemists, Afiliated East West Press, 1969

LEARNING OUTCOMES

After the completion of this course students will be able to understand about

- The principles and applications of group theory
- Various theories of chemical reaction kinetics
- Kinetics of different types of reactions
- Applications of group theory to molecules
- Thermodynamic properties of various components
- Different types of catalysis
- Surface phenomena and various adsorption isotherms
- Surface chemistry and its applications to heterogeneous catalysis

SEMESTER-I **HOURS/WEEK: 6**
CHE514CP **CREDITS: 3**

ORGANIC CHEMISTRY PRACTICAL - I

- To learn the qualitative analysis of an organic mixture
- To know the preparation of organic compounds

Separation of Mixtures

Mixtures containing two components are to be separated (Pilot separation) and purified (bulk separation) – The physical constants are to be reported - analysis with minimum one Confirmation test for each group (whenever possible, the UV-Vis and IR Spectra may be recorded for characterization of functional groups)

Column Chromatography

Separation of *o*- and *p*-nitrophenols and similar systems. Identification by Thin layer chromatography – The physical constants are to be reported.

Preparations – (Two stages)

1. Acetanilide to *p*-bromoacetanilide to *p*-bromoaniline.
2. Acetanilide to *p*-nitroacetanilide to *p*-nitroaniline.
3. Preparation of Cu_2Cl_2; 2-chlorobenzoic acid from anthranilic acid.
4. Benzoin to benzil to benzilic acid.
5. Benzophenone to benzopinacol to benzopinacolone.

Demonstration only

About 6-8 preparations (involving two or more than two steps) involving the following representative reactions

1. Esterification and saponification
2. Oxidation
3. Hydride reduction
4. Nucleophilic substitution
5. Cycloaddition reaction
6. Condensation reaction
7. Aromatic electrophilic substitution
8. Heterocyclic synthesis

Reference Books

1. J. Mohan, Organic Analytical Chemistry, Theory and Practice, Narosa, 2003.
2. V.K. Ahluwalia, P. Bhagat, R. Aggarwal, Laboratory Techniques in Organic Chemistry, I.K. International, 2005.
3. N.S. Gnanaprakasam, G. Ramamurthy, Organic Chemistry Lab Manual, S.V. Printers, 1987.
4. A.I. Vogel, A.R. Tatchell, B.S. Furniss, A.J. Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Prentice Hall, 1996.

LEARNING OUTCOMES

After the completion of this course, students will be able to

- To familiarize the solubility nature of organic substances of different functional group.
- Identify the number of compounds by thin layer chromatography
- To expertise in separating and purifying the components of a mixture ny column chromatography
- To learn the pilot separation of mixtures.
- To familiarize the systematic producers organic substances analysis
- To learn two stage preparation involving molecular rearrangement
- To understand the techniques involving drying and recrystallization by various method
- To expertise the various techniques of preparation and analysis of organic substances

SEMESTER-I **HOUR/WEEK: 6**
CHE515CP **CREDIT: 3**

INORGANIC CHEMISTRY PRACTICAL - I

OBJECTIVES

- To learn the Semi-micro qualitative analysis and quantitative analysis
- To learn Preparations and characterization of Co-ordination Complexes.

1. **Semimicro qualitative analysis** of a mixture of salts containing two common cations (Pb, Bi, Ca, Cd, Fe, Cr, A1, Co, Ni, Mn, Zn, Ba, Sr, Ca, Mg, NH_4+) and two less common cations (W, Tl, Se, Te, Mo, Ce, Th, Zr, Ti, V, U,Li).
2. **Preparations and Characterization of Co-ordination Complexes**

1. Tris(thiourea)copper(I) sulphate
2. Tetramminecopper(II) sulphate
3. Pentathioureadicuprous nitrate
4. Potassium trioxalatoferrate
5. Potassium trioxalatoalumiate
6. Potassium trioxalatochromate
7. Cis-Potassium dioxalatodiaquochromate
8. Hexathioureaplumbem nitrate
9. Hexamminecobalt(III) chloride
10. Ferrocene and its simple derivatives

Spectral characterization of the above mentioned synthesized complexes.

3. Demonstration only

Quantitative Analysis

a) Redox titrations : Fe(II) vs. Ce(IV) , Fe(II) vs. dichromate, NO_2^- vs. Ce(IV)

b) Spectrophotometric methods of analysis : Fe(II), Cu(II).

Reference Books

1. V.Ramanujam, Inorganic Semi Micro Qualitative Analysis, National Pubs. 1988.

2. A.I. Vogel, Text Book of Quantitative Inorganic Analysis, 5th Ed., Longman, 1989.

LEARNING OUTCOMES

After the completion of this course, students will be able to learn

- The semi-micro qualitative analysis.
- To familiarize the test involving indentification of special elements
- Preparations of Co-ordination Complexes.
- Semi-micro qualitative analysis of a mixture of salts containing two common two less common cations
- To learn the confirmatory test for various cations
- To understand the techniques involving drying and recrystalliation of synthesized complexes
- To expertise the various techniques of preparation and increase the yield of the complexes
- Spectral characterization of the synthesized complexes.

SEMESTER-I **HOUR/WEEK: 6**

CHE516CP **CREDIT: 3**

PHYSICALCHEMISTRY PRACTICAL – I

Any ten experiments from the following experiments (to be decided by the course teacher):

1. Kinetics – Acid Hydrolysis of Ester – Comparison of strength of acids.
2. Kinetics – Acid Hydrolysis of Ester – Determination of Energy of Activation (E_a).
3. Kinetics – Persulphate – Iodide Reaction – Determination of order, effect of Ionic strength on rate constant.
4. Adsorption – oxalic Acid\Acetic Acid on charcoal using Freundlich isotherm.
5. Conductometry – Acid – alkali titrations.
6. Conductometry – precipitation titrations.
7. Conductometry – Determination of dissociation constant of weak acids.
8. Verification of Onsager equation – conductivity method.
9. Determination of degree of hydrolysis and hydrolysis constant of a substance.
10. Distribution Law – Study of Association of Benzoic Acid in Benzene.
11. Distribution Law – Study of iodine – Iodide equilibrium.
12. Conductometry - Displacement titrations.
13. Conductometry – Solubility product of sparingly soluble silver salts.
14. Kinetics – Saponification of Ester – Determination of E_a by conductometry.
15. Polymerization – Rate of polymerization of acrylamide.
16. To verify the Beer-Lambert's law and determine the concentration of unknown from absorption measurement.

Non-Instrumental: (Demonstration only)

a. Determination of surface excess of amyl alcohol or TX-100 surfactant by Capillary rise method.
b. Statistical treatment of experimental data.
c. Determination of molecular weight by steam distillation. 4) Glycerol radius by viscosity.

Reference Books

1. B.P. Levitt, Ed., Findlay`s practical Physical Chemistry, 9th Ed., Longman, 1985.
2. J.N. Gurtu, R. Kapoor, Advanced Experimental Chemistry, Vol.I, S.Chand& Co., 1987.

LEARNING OUTCOMES

After the completion of this course, students will be able

- To prepare for each experiment by studying lab handouts and links therein
- To know about the safety requirements and lab skills to perform physico-chemical experiments
- To appreciate the modern problems and scientific controversies in physical chemistry
- To design and perform experiments to determine the rate, order and activation
- To understand the non-instrumental physical chemistry experiments
- To demonstrate acid-base and precipitation titrations by conductometry and to verify Onsager equation
- To find out the solubility product of sparingly soluble salt by conductometry.
- To verify Beer-Lambert's law and determine the unknown concentration
- To calculate the rate of polymerization

SEMESTER-II **HOURS/WEEK: 6**
CHE521CC **CREDITS: 5**

ORGANIC CHEMISTRY – II

OBJECTIVES

- To study electrophilic and nucleophilic substitution and their mechanisms
- To study addition and elimination reactions and their mechanism
- To study the concept of pericyclic and photochemical reaction

UNIT I

1. Electrophilic Substitution Reactions

Aromatic electrophilic substitution: Orientation, reactivity and mechanisms – Synthetic applications – Substitutions in thiophene and pyridine –Quantitative treatment of the structural effects on reactivity – Substituents effect – Origins of Hammett equation – Principles of Hammett correlation – Effect of structure on reaction mechanisms Hammett parameters; σ and ρ, modified forms of Hammett equation – Taft Equation.
Aliphatic electrophilic substitution: S_E1, S_E2, S_Ei mechanisms – Simple examples only.

UNIT II

2. Nucleophilic Substitution Reactions

Aliphatic nucleophilic substitution – Mechanisms; S_N1, S_N2, S_Ni – stereochemical aspects of nucleophilic substitution reactions – Ion-pairs in S_N1 mechanism – Neighbouring group participation – Non-classical carbocations – Substitutions at allylic and vinylic carbons – Reactivity: Effect of structure, nucleophile, leaving group and solvent – Ambident substrates and nucleophiles – Aromatic nucleophilic substitution: Mechanisms; S_NAr, Benzyne, S_N1.

UNIT III

3. Addition and Elimination Reactions

Addition to carbon-carbon multiple bonds: Electrophilic, nucleophilic and free radical additions – Orientation of the addition – Stereochemical factors influencing the addition of bromine and hydrogen bromide, hydroxylation, 1,2-dihydroxylation – Hydroboration leading to formation of alcohols – Oxidation – Sharpless asymmetric epoxidation and ozonolysis. Addition to carbonyl and conjugated carbonyl systems – Mechanism – Grignard reagents – 1,2 and 1,4-additions (dimethyllithiumcuprate type).
Addition to carbon-oxygen double bond: A study of benzoin, Knovenagel, Stobbe and Darzen-glycidic ester condensation reactions.
Elimination Reactions: Mechanisms; E1, E2, E1cB – Stereochemistry of elimination, Hofmann and Zaitsev rules – Pyrolytic *cis* elimination, Chugaev reaction – Cope elimination – Bredt's rule.

UNIT IV

4. Organic Photochemistry

Fundamental concepts – Energy transfer – Types of excitation – Quantum yield - Photosensitization – Photochemistry of carbonyl compounds: Norrish Type I, II and related reactions – Parterno-Büchi reaction – Photochemistry of unsaturated carbonyl compounds: Photodimerisation - Photochemistry of alkenes, dienes and aromatic compounds – Photorearragement of enones and dienones - Photo-Fries rearrangement – Di-π-methane rearrangement – Photoreduction and Photooxidation – Photo-substitution reactions; de Mayo, Barton and Hofmann-Loffler-Freytag reactions – Photochromism - Chemistry of vision.

UNIT V

5. Pericyclic Reactions I

Molecular orbitals in conjugated polyenes, ions, radicals - Orbital symmetry – Electrocyclic reactions: Con-rotatory and Dis-rotatory - Frontier molecular orbital method – Correlation diagram – Selection rules - Cycloaddition reactions: FMO method - Correlation diagram – Selection rules – Chelotropic reactions - 1,3-Dipolar cycloaddition reactions - Sigmatropic rearrangement: 1,3- and 1,5-hydrogen shifts - FMO method - Selection rules – Cope and Claisen rearrangements – Group transfer reactions: ene reactions including diimide – Problems in each section.

UNIT VI (Not for final examination)

6. Pericyclic Reactions II

Theory of Concerted Reactions- – the aromatic transition state concept – general rule for pericycle reactions - Definition – thermal electrocyclic reactions – photochemical electrocyclic reactions – metal catalysed electrocyclic reactions- Diels – Alder reaction – The retro diels – alder reaction – Retro – 1,3 – dipolar cyclo additions- 2,3, - sigmatropic changes – ylide rearrangements – photochemical re-arrangements– Problems in each section.

Text and Reference Books

1. J. Clayden, N. Greeves, S. Warren, Organic Chemistry, 2nd Ed., Oxford University Press; 2012.
2. T.H. Lowry, K.S. Richardson, Mechanism and Theory in Organic Chemistry, Addison-Wesley, 1998.
3. J. March, M.B. Smith, Advanced Organic Chemistry: Reactions, Mechanisms and Structure; 6th Ed., Wiley, New York, 2007.
4. R.K. Bansal, Organic Reaction Mechanisms, New Academic Science, 2012.

5. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry; Parts A & B, 5th Ed., Springer, Germany, 2007.
6. H.O. House, Modern Synthetic Reactions, 2nd Ed., W. A. Benjamin, New York, 1998.
7. S. Kumar, V. Kumar, S.P. Singh, Pericyclic Reactions: A Mechanistic and Problem-Solving Approach; Academic Press: New York, 2016.
8. I. Fleming, Pericyclic Reactions, Oxford Science Publications, Cambridge, 1998.
9. J. Kagen, Organic Photochemistry: Principles and Applications, Academic Press: New York, 1993.
10. J. D. Coyle, Introduction to Organic Photochemistry, John Wiley and Sons, Great Britain, 1989.
11. V. Ramamurthy, S. S. Kirk, Organic and Inorganic Photochemistry, Vol, 2, Marcel Dekkar Inc., New York, 1998.
12. J. Singh and J. Singh, Photochemistry and Pericyclic Reactions, New Age International (P) Ltd., New Delhi, 2007

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Orientation, reactivity and mechanisms of electrophilic substitution reactions
- Aliphatic and aromatic nucleophilic substitutions reactions
- Neighboring group participation and effect of structure, leaving group and solvent on reactivity
- Addition and elimination reactions and their mechanism
- Various types of addition and elimination reactions
- Fundamental concepts of organic photochemical reactions
- Understand the chemistry of vision by photochemistry
- Pericyclic reactions, correlation diagrams, rearrangements and related problems

SEMESTER-II **HOURS/WEEK: 6**
CHE522CC **CREDITS: 5**

INORGANIC CHEMISTRY - II

(Bio-Inorganic and Organometallic Chemistry)

OBJECTIVES

- To understand the role of metal ions in biological process
- To learn the fundamentals of medicinal bio-inorganic chemistry
- To learn the basics of organometallics, reaction mechanisms and catalysis

UNIT I

1. Introduction to bioinorganic chemistry

Essential and trace elements and their role in biological process, Porphyrins, corrin and chlorin as Biological ligands, structural models. Vitamin B_{12}-Reactions of the alkyl cobalamins, One-electron Reduction and Oxidation – Co-C Bond Cleavage – coenzyme B_{12}, Ionophores (examples), sodium/potassium transfer across the membrane.

2. Bioenergetics and ATP Cycle

DNA polymerization, glycolysis (glucose to pyruvate conversion) and glucose storage, chlorophylls, Photosystems I and II in cleavage of water, Involvement of Oxygen evolving complex in oxidation of water to O_2

UNIT II

3. Heme and Non-heme Proteins

Oxygen transport and storage: Structure and functions of Hemoglobin, Myoglobin, Hemerythrin and Hemocyanin, Bohr Effect, synthetic models. Importance of 2,3-diphosphoglycerate, CO and CN poisoning, hematin formation

Classification of copper proteins and examples: blue copper proteins (azurin and plastocyanin) and Superoxide dismutase

4. Electron Transfer in Biology

Structure and functions of electron transfer proteins such as Iron-sulphur proteins (Ferredoxins, Rubredoxin and Rieske's protein) and Cytochromes (classification and Oxygen activation using Cytochrome C Oxidase)– synthetic models, siderophores.

UNIT III

5. Nickel and Molybdenum containing Enzymes

Structure and functions of Urease, Hydrogenases, biological nitrogen fixation using molybdenum nitrogenase- spectroscopic and other evidences, other nitrogenase model systems.

6. Metals in Medicine: cis-platin, and its mode of action, side effects;

Gold containing drugs as anti- rheumatic agents and their mode of action - Lithium in Pschycopharmocological drugs.

UNIT-IV

7. Organometallics : Basic Concepts

Hapticity, ligand classification, synthesis and structure – The 18 electron rule – limitations and applications–preparation, properties, structure and bonding in metal carbonyls, nitrosyls, metal olefins, acetylenes, metallocene-ferrocene and Half – sandwhich compounds-arene complexes, Isolobal analogy and its applications.

UNIT V

8. Organometallic Chemistry: Reactions and Catalysis by Organometallics

Organometallic reactions-Ligand association and dissociation, oxidative addition and reductive elimination, Insertion reactions, reactions of coordinated ligands in organometallics. Reaction mechanism for hydrogenation, hydroformylation (oxo process), olefin oxidation (Wacker process) and carbonylation of methanol, epoxidation, alkene metathesis, Ziegler-Natta catalyst.

UNIT VI (Not for final examination)

9. Medicinal Bioinorganic Chemistry

Bioinorganic Chemistry of quintessentially toxic metals. Lead, Cadmium, Mercury, Aluminum, Chromium, Iron, Copper, Plutonium. Detoxification by metal chelation. Drugs that act by binding at the metal sites of Metalloenzymes. Chemotherapy-Chemotherapy with compounds of certain non-essential elements. Cytotoxic compounds of other metals - Molecular channels and transport processes.

Text and Reference Books

1. J. E. Huheey, *Inorganic Chemistry;* 4th Ed., Harper & Row Publishers, Singapore, 2006. (All Units)
2. F.A Cotton, G. Wilkinson, *Advanced Inorganic Chemistry*, 6th Ed., WileyInterscience Publication, John Wiley & Sons, New York, USA, 1999. (All Units)
3. I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine *Bioinorganic Chemistry* University Science Books, USA, 1994
4. S. J. Lippard, J.M. Berg, *Principles of Bioinorganic Chemistry* , Panima Publishing Company, New Delhi, 1997. (Units I-III)
5. D. E. Fenton, *Oxford Chemistry Primer Series: Biocoordination Chemistry*, Oxford University Press, 1995
6. W. Kaim, B. Schewederski, A. Klein *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, John Wiley & Sons, 2nd Edn. 2013. (Units I-III)
7. *Bioinorganic Chemistry,* Chem. Education, 62, No. 11, 1985. (Units I-III)
8. A. K. Das, *Bioinorganic Chemistry*, Books and Allied Ltd. Kolkatta, 2016. (Units I-III)

9. P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn. Chapman and Hall, 1988. (Units IV and V)
10. R. H. Crabtree, *the Organometallic Chemistry of the Transition Metals*, 4th Edn. Wiley – Interscience, 2005. (Units IV and V)
11. A. J. Elias, B. D. Gupta, *Basic Organometallic Chemistry* 2nd Edn. University Press, 2013. (Units IV and V)
12. J.P. Collman, L.S. Hegedus, J.R. Nortan, R.G. Finke, *Principles and Applications of Organotransition Metal Chemistry*, University Science Books, 1980. (Units IV and V)

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- The role of metal ions in biological process
- Basic concepts of organometallic chemistry in catalysis
- Basic units of organometallic compounds present inside the human body
- Bioenergetics and ATP cycle in DNA polymerization, glycolysis
- Mechanism of photosynthesis and electron transport in biology
- Structure and function of heme and non-heme proteins, bio-enzymes
- Fundamentals of bio-inorganic chemistry
- Metal based drugs in cancer, rheumatoid arthritis and psychopharmacology

SEMESTER-II **HOUR/WEEK: 6**

CHE523CC **CREDIT: 5**

PHYSICAL CHEMISTRY - II

OBJECTIVES

- To understand the fundamentals of quantum chemistry and its applications to simple systems
- To learn the basics of phase rule, colloids and micelles
- To learn the principles of photophysics and electrochemistry

UNIT I

Basic Mathematics and Fundamentals of Quantum Chemistry

Basic Mathematics- Exponential functions, vectors, matrices, determinants, differentiation, Integration and differential equations. Introduction to quantum mechanics - Black body radiation, photoelectric effect, de Broglie equation and its verification, Interpretation of Bohr's first postulate in terms of wave nature of electron, Heisenberg Uncertainty principle; Setting up the Schrödinger equation, operators, algebra of operators, linear operators, setting up operators of linear momentum, angular momentum, kinetic energy and total energy of systems.

UNIT II

Quantum Mechanics of Simple Systems

Writing the Hamiltonian for H and He atoms- eigen functions and eigen values, proving that linear momentum and angular momentum operators are linear, Hermitian operator and its properties, commutator theorem and its converse, Expansion theorem; Postulates of quantum mechanics. The Schrödinger wave equation- particles in 1D and 3D boxes, harmonic oscillator, rigid rotator, Hydrogen atom, Hydrogen orbital - Time dependent Schrödinger wave equation- Approximation methods - Perturbation Theory (first order and non-degenerate), The Variation method, linear variation principle, Helium - Hartree-Fock self-consistent field method.

UNIT III

Quantum Theory

Approximate methods of solving the Schrodinger equation – The perturbation and variation methods – Angular momentum– spin orbit interaction – vector model of the atom – term symbols - Pauli exclusion principle Slater determinant. Atomic Structure Calculation - distortion of the box and Jahn-Teller effect, quantum numbers, zero-point energy, finite potential barrier – tunneling.

UNIT IV

Electrochemistry-Ionics

Mean ion activity and activity coefficient of electrolytes in solution - ion association – ionicstrength - Debye-Hückel theory and Debye-Hückel limiting law - its validity and limitations -strong and weak electrolytes - Debye theory of electrolytic conductance - Debye-Hückel- Onsager equation - verification and limitations - electrochemical cells and applications of standard redoxpotentials.

UNIT V

Phase rule, colloids and micelles

Phase rule: Three component systems – representation by triangular diagrams, systems of three liquids – formation of one pair of partially miscible liquids, formation of two pairs of partially miscible liquids, formation of three pairs of partially miscible liquids – solid-liquid phases, Eutectic systems.

Colloids: Distinction between suspension, colloidal solutions and true solutions – lyophilc and lyophobic colloids – Tyndall effect – stability of colloids – coagulation – emulsions – various types. Micelles: Surfactant (amphipathic molecules) – micellization - critical micelle concentration – size of micelle – aggregation number – Thermodynamics of micellization– reverse micelles.

UNIT VI (Not for final examination)

Principles of Photophysics

Absorption of light by molecules – Reaction paths of electronically excited molecules - Fluorescence and phosphorescence – Jablonski diagram – Physical properties of the electronically excited molecules: Excited state dipole moments, Excited state pKa and redox potentials – Life timeof excited state molecules-TCSPC- Stern-Volmer equation and its application – Photoinduced electron transfer, free energy dependence of electron transfer on rate –FRET- Fluorescence quantum yield.

Text Books

1. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998.
2. A.K. Chandra, Introductory Quantum Chemistry, 4th Ed,. Tata McGraw Hill, 2009.
3. C.H. Hamann, A. Hammett, W. Vielstich, Electrochemistry, Wiley-VCH, 1998.
4. A.J. Bard, L.F. Pahlkner, Electrochemical methods – Fundamentals and applications, 2nd Ed., Wiley-VCH, 1998.
5. J. Albery, Electrode kinetics, Clarendon Press, Oxford Chemical Series, 1979.
6. J. N. Gurtu, K.S. Gurtu, Phase rule, PargatiPrakashan, 1971.
7. B.K. Sharma, Colloid Chemistry,Goel Publishing House, 1975.
8. M.J. Vold, R.D. Vold, Colloid Chemistry, The science of Large molecules, small particles and surfaces. Chapman and Hall, 1965.
9. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.
10. R.J. Hunter, Foundations of Colloid Sciences, Vol. 1 and 2, Clarendon Press, 1995.

11. J.R. Lakowicz, Principles of fluorescence spectroscopy, Springer, 2006.
12. K.K. Rohatgi – Mukherjee, Fundamentals of Photochemistry, New Age International, 2000.

Reference Books

1. G. Doggett, B.T. Sutcliffe, Mathematics for chemistry, Addison Wesley Longman, 1995.
2. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998
3. F.L. Pillar Elementary Quantum Chemistry, McGraw Hill 1968
4. J.P. Lowe, K.A.Peterson, Quantum Chemistry, 3rd Ed, Elsevier, 2006.
5. I.N. Levine, Quantum Chemistry, 5th Ed, Prentice Hall, 2000.
6. P.W. Atkins, Molecular Quantum Mechanics,2nd Ed., Oxford Univ. Press, 1987.
7. J. Goodisman, Contemporary Quantum Chemistry, Planum Press, 1977.
8. R.K. Prasad, Quantum Chemistry,New Age International Publishers, 1997.
9. H. Metiu, Quantum Mechanics, Taylor & Francis, 2006.
10. J.O. Bockris and A.K.N. Reddy, Modern Electrochemistry, 2nd Ed., Springer, 2006.
11. L.I. Anthrapov, Theoretical Electrochemistry, Mir Publishers, Moscow, 1972.
12. P.H. Rieger, Electrochemistry, Prentice-Hall, Inc, 1987.
13. N.J. Turro, Molecular Photochemistry, W. A. Benjamin, 1966.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- The fundamentals of quantum chemistry and its applications to simple systems
- Principles of photophysics and electrochemistry
- Applications of basic Mathematics to Quantum Chemistry
- Black body radiation, photoelectric effect, de Broglie equation and its verification
- Application of quantum mechanics to simple systems
- Basic concepts of electrochemistry including electrolytes, Debye-Huckel theory of electrolytic conductance, verification and limitations of Debye-Hückel- Onsager equation
- Applications of electrochemical cells and standard redox potentials.
- The fundamentals of Phase rule, colloids and micelles

SEMESTER-II **HOURS/WEEK: 6**
CHE524CP **CREDITS: 3**

ORGANIC CHEMISTRY PRACTICAL - II

OBJECTIVES

- To learn the separation, estimations and purification of an organic compounds
- To know the preparation and isolation of organic compounds.

1. Estimation

1. Estimation of Aniline
2. Estimation of Phenol
3. Estimation of Methyl ketones
4. Estimation of Glucose
5. Estimation of Hydroxyl group
6. Estimation of Nitro group

2. Preparation and Isolation

1. Aniline to tribromoaniline to tribromobenzene
2. Methyl benzoate to methyl-*m*-nitrobenzoate to methyl-*m*-nitrobenzoic acid
3. Methyl salicylate to salicyclic acid to acetyl salicyclic acid
4. Chlorobenzene to dinitrochlorobenzene to 2,4-dinitrophenylhydrazine
5. Hydroquinone to *p*-benzoquinone to 5-hydroxy-1,3-benzoxathiaole to 5-acetoxy-1,3-benzoxathiaole-2-one
6. Extraction of Caffeine from tea leaves
7. Extraction of Eugenol from clove

3. Purification techniques (Demonstrations)

a) Purification of solvents and reagents using techniques like crystallization, distillation, steam distillation, vacuum distillation, drying and storage of solvents, sublimation etc. b) Chromatography: TLC, Column, paper c) Solvent extraction using soxhlet extractor

4. Three component mixture separation using ether.
(8 mixtures minimum including amino acid)

Reference Books

1. J. Mohan, Organic Analytical Chemistry, Theory and Practice, Narosa, 2003.
2. V.K. Ahluwalia, P. Bhagat, R. Aggarwal, Laboratory Techniques in Organic Chemistry, I.K. International, 2005.
3. N.S. Gnanaprakasam, G. Ramamurthy, Organic Chemistry Lab Manual, S.V. Printers, 2000.
4. A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Prentice Hall, 1996.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- The solubility nature of organic substances of different functional group.
- Estimation of organic compounds
- Estimation of hydroxyl groups in natural products and antioxidants
- Preparation, separation and purification of organic compounds
- Isolation of organic compounds
- Extraction of caffeine from tea leaves
- Extraction of eugenol from clove
- Conversion of functional groups in organic preparations

SEMESTER-II **HOUR/WEEK: 6**
CHE525CC **CREDIT: 3**

INORGANIC CHEMISTRY PRACTICAL - II

OBJECTIVES

- To learn the Titrimetric and Gravimetric analysis.
- To learn the Preparations and characterization of compounds.
- To learn spectrophotometric method of estimation

1. Volumetric and gravimetric analysis of a solution containing two cations

1. Copper and Nickel
2. Copper and Zinc
3. Ferrous and Ferric ions
4. Barium and Calcium

2. Simple Volumetric Titrations

EDTA Titrations: Calcium(II), Magnesium(II), Zinc(II), Iron(II), Iron(III), Copper(II), Nickel(II).

3. Total hardness of a sample of hard water

4. Spectrophotometric estimation of three metal ions.

5. Photometric titration of systems such as: a) Cu^{2+} - EDTA b) Fe^{2+} - Sulphosalicylic acid c) Co^{2+} - R-nitroso salt.

Reference Book

1. A.I. Vogel's, Quantitative Inorganic Analysis, 5th Ed., Prentice Hall, 1996.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Principles of titrimetry and gravimetry analysis.
- Volumetric and gravimetric analysis of cations and anions
- Set up glassware and apparatus to conduct experiments without error
- Preparations and characterization of compounds.
- Spectrophotometric method of estimation
- Volumetric and gravimetric analysis of a solution containing two cations
- Hardness of a sample of hard water
- Spectrophotometric estimation of three metal ions.

SEMESTER-II **HOUR/WEEK: 6**
CHE526CP **CREDIT: 3**

Physical Chemistry Practical– II

OBJECTIVES

- To learn the determination of molecular weight experiments
- To know the potentiometric experiments

Any ten experiments out of the following experiments (to be decided by the course teacher):

1. Determination of molecular weight of substances by cryoscopy.
2. Determination of Molecular weight of substances by Transition Temperature method
3. Determination of molecular weight of substances by Rast method.
4. Determination of Critical Solution Temperature of phenol water system and effect of impurity on SCT.
5. Determination of integral and differential heat of solutions by colorimetry.
6. Study of phase diagram of two components forming simple eutectic.
7. Study of phase diagram of two components forming a compound.
8. Study of phase diagram of three components system (Acetic acid, Benzene, and water).
9. Potentiometric titrations – Acid alkali titrations.
10. Potentiometric titrations – preciptation titration.
11. Potentiometric titrations – Redox Titrations.
12. Poentiometry – Determination of dissociation constant of week acids.
13. Potentiometry – Determination of solubility of silver salts.
14. Potentiometry – Determination of activity and activity coefficients of Ions.
15. pH titration of ortho-phosphoric acid.
16. Determination of the acid and base dissociation constant of an amino acid and hence the isoelectric point of the acid by pH method.
17. Analysis of a binary mixture by colorimetry
18. Kinetic decomposition of diacetone alcohol by dilatometry
19. Non-Instrumental Determination of molecular weight by steam distillation. 4) Glycerol radius by viscosity. 5) Partial Molar Volume (Polynometry) Determination of the densities of a series of solutions and to calculate the molar volumes of the components. 6) Surface area analysis by BET method e.g. industrial pigment 7) Determination of surface excess of amyl alcohol or TX-100 surfactant by Capillary rise method.

Reference Books

1. B.P. Levitt, Ed., Findlay`s Practical Physical Chemistry, 9th Ed., Longman, 1985.
2. J.N. Gurtu, R. Kapoor, Advanced Experimental Chemistry, Vol.I, S.Chand& Co., 1987.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Determination of molecular weight by various methods
- Determination of integral and differential heat of solutions by colorimetry.
- Phase diagram of two components forming simple eutectic and forming components
- pH titration of ortho-phosphoric acid.
- Determination of solubility of silver salts
- Determination of dissociation constant of week acids.
- Determination of activity and activity coefficients of ions
- Redox titrations by potentiometry

SEMESTER-III **HOURS/WEEK: 6**
CHE531CC **CREDITS: 5**

ORGANIC CHEMISTRY – III

OBJECTIVES

- To understand the basic concepts of asymmetric synthesis
- To study pericyclic reactions and its applications
- To study the concepts of heterocyclic chemistry and its applications
- To study the concepts of named reactions and its applications
- To study reagents and their mechanisms of reactions

UNIT I

1. Heterocycles

Nomenclature: Trivial, systematic and replacement nomenclatures – Chemistry of non-aromatic heterocycles: Oxiranes – Thiiranes – Aziridines – Azetidines – Tetrahydrofurans – Pyrrolidines – Tetrahydropyrans – Piperidines – Ring synthesis and reactivity of the following aromatic heterocycles: Oxazoles – Thiazoles – Imidazoles – Isooxazoles – Isothiazoles – Pyrazoles – Triazoles – Pyrimidines – Purines – Triazines.

UNIT II

2. Named Reactions and Strategic Applications in Organic Synthesis

Bamford-Stevens Reaction – Barton-McCombie Reaction (Barton Deoxygenation) – Baylis-Hillman Reaction – Biginelli Reaction – Corey-Chaykovsky Reaction – Enamines and selective alkylation (mono and di) via enamine reactions – Henry Reaction – Hosomi-Sakurai Reaction – Hunsdiecker Reaction – Julia Olefination and its modifications – Mitsunobu Reaction – Mukaiyama Aldol Addition – Nazarov Cyclization – Peterson Olefination – Prevost Reaction – Prins Reaction – Staudinger Reaction – Ugi Reaction – Weinreb Ketone Synthesis – Wittig reaction and its modifications – Yamaguchi Macrolactonization. Palladium based reactions: Fukuyama Coupling – Heck Reaction – Hiyama Coupling – Sonogashira Coupling– Stille Coupling – Suzuki Coupling – Tsuji-Trost Reaction.

UNIT III

3. Reagents in Organic Synthesis

Oxidation: Jones reagent, PCC, PDC, MnO_2, Tempo, DMSO with DCC, Ac_2O or oxalyl chloride, IBX, Dess-Martin periodinane, DDQ, Lead tetraacetate, SeO_2.

Reduction: Catalytic hydrogenation (metal/H_2), Homogeneous hydrogenation (Wilkinson's catalyst), Hydride transfer reagents [$NaBH_4$ and LAH (with or without co-reagents), $NaCNBH_3$, $NaBH(OAc)_3$, B_2H_6, DIBAL-H, Li(*t*-BuO)$_3$AlH, K & L-selectrides], trialkylsilanes, dissolving metal reductions, Reductions with hydrazines, Baker's yeast.

Miscellaneous: LDA – Phase transfer catalysis (PTC)

UNIT IV

4. Asymmetric Synthesis

Basic principles of Asymmetric synthesis – Enanatioselective and diastereoselective – Analytical methods for determining enantiomeric excess. Asymmetric synthesis on chiral substrate: Nucleophilic addition to α-chiral carbonyl compounds; Prediction of stereochemistry – Cram's rule and related modifications. Asymmetric synthesis using chiral reagents: Chiral modification of lithium aluminum hydride – BINAL-H – Application in reduction of prochiral ketones; oxazaborolidines. T.S model. Asymmetric Michael addition to α,β-unsaturated carbonyl compounds – T.S model. Chiral lithium amides, enantioselective deprotonation. Asymmetric synthesis using chiral auxiliary: Chiral auxiliaries derived from proline, champhor and menthol. Asymmetric synthesis using chiral catalysts: Asymmetric alkylation and allylation of carbonyl compounds – Noyori's BINAP – Jacobson catalyst – Evans catalyst.

UNIT V

5. Advanced Spectroscopy I: UV –Vis, IR and MS

5.1. UV-Visible Spectroscopy

Introduction – Instrumentation – sample handling techniques – Woodward–Fieser and Scott rules for conjucated dienes and polymers, ketones, aldehydes, ∝,β-unsaturated acids, esters, nitriles, and amides – Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives – Study of steric effect in aromaticity.

5.2. Infrared Spectroscopy

Introduction – Instrumentation – Sampling techniques – Factors influencing group frequencies – Both internal and external – Quantitative studies – Hydrogen bonding(intermolecular and intramolecular).

5.3. Mass Spectrometry

Introduction – Instrumentation – Resolution, EI and CI methods – Base peak, isotopic peaks, metastable peak, parent peak – Determination and use of molecular formula – Recognition of molecular ion peak – FAB – Fragmentation: General rules – Pattern of fragmentation for various classes of compounds – McLafferty rearrangement – Importance of metastable peaks.

5.4. PMR: Fundamentals of NMR, CW and FT-NMR, factors affecting chemical shift, integration coupling (1st order analysis)- Introduction of CMR and mass spectrometry

UNIT VI (Not for final examination)

6. Problems based on joint application of UV, IR, PMR, CMR, and Mass. (Including reaction sequences)

Text and Reference Books

1. J. D. Morrison, Asymmetric Synthesis; Vols 1-5, 1st Ed., Wiley-VCH, 2000.
2. R. Noyori, Asymmetric Catalysis in Organic Synthesis, Wiley, 1996.
3. I. Ojima, Catalytic Asymmetric Synthesis, Wiley, 2010.
4. H.B. Kagan, Aymmetric Synthesis, 1st Ed., Thieme Medical Publishers, 2009.
5. H.O. House, Modern Synthetic Reactions, 2nd Ed., W. A. Benjamin, 1998.

6. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry, Parts A & B, 5th Ed., Springer, 2007.
7. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Ed., 2004
8. T. L. Gilchrist, Heterocyclic Chemistry, 3rd Ed., Prentice Hall, 1997.
9. J.A. Joule, K. Mills, Heterocyclic Chemistry, 4th Ed., Blackwell Publishing, 2007.
10. T. Eicher, S. Hauptmann, 2nd Ed., Wiley-VCH, 2003.
11. R.K. Bansal, Heterocyclic chemistry, Anshan Ltd, 2008.
12. R.K. Mackie, D.M. Smith, Guide Book to Organic Synthesis, 3rd Ed., Prentice Hall, England 2000.
13. L. Kurti, B. Czako, Strategic Applications of Named Reactions in Organic Synthesis, Elsevier, 2005.
14. A. Hassner, C. Stumer, Organic Synthesis Based on Name and Unnamed Reactions, Elsevier Science Ltd., UK, 1994.
15. G. Brahmachari, Organic Name Reactions: A Unified Approach, Alpha Science Intl. Ltd, 2006.
16. Also refer: http://www.organic-chemistry.org/; http://www.organicworldwide.net.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Synthesis and importance of chemistry of heterocycles.
- Important naming reactions and their applications to organic synthesis.
- Important of reagents in organic synthesis
- Mechanisms of naming reactions.
- Basic concepts of asymmetric synthesis.
- Basic concepts of advanced spectroscopic techniques.
- Instrumentation of spectrometers.
- Application of spectroscopy in the structural elucidation of organic compounds.

SEMESTER-III **HOURS/WEEK: 6**
CHE532CC **CREDITS: 5**

INORGANIC CHEMISTRY- III

(Physical Methods in Inorganic Chemistry)

OBJECTIVES

- To learn the spectral characterization of inorganic compounds
- To study the structural chemistry using single crystal X-Ray Diffraction

UNIT I

1. Electronic Spectroscopy

Spin-orbit coupling and effect of distortion on spectra-Terms, states, microstates and energy levels for d^1 – d^9 ions, Electronic spectra of octahedral and tetrahedral complexes of d^1 – d^9 ions, Orgel and Tanabe-Sugano diagram for d^1-d^9 states, selection rules and its exemptions (allowed and forbidden transitions), group theoretical approach to selection rules. nephelauxatic effect, Charge transfer spectra, Evaluation of 10Dq and β for octahedral nickel and tetrahedral cobalt complex, electronic spectra of $[Ru(bpy)_3]^{2+}$and its application in photo oxidation of water.

UNITII

2. Infrared and Raman Spectroscopy

Vibrations in simple molecules (H_2O, CO_2) and their symmetry notation for molecular vibrations, group vibration concept and its limitations. Effect of coordination on ligand vibrations, uses of groups vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide. Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, structure and geometry.

Raman Spectroscopy principle, selection rule, combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^-.

UNIT III

3. Multinuclear NMR Spectroscopy

Examples for different spin systems such as ^1H, ^{19}F, ^{31}P, ^{13}C,chemical shifts and coupling constants (J)involving above nuclei.

^1H NMR of inorganic hydrides (SiH_3PH_2, BH_4^-, $[HRh(CN)_5]^{3-}$, $[H_2Fe(CO)_4]$);^{19}F spectra (of ClF_3, ClF_5, TiF_4, R_2PF_3, BrF_5, SF_4, PF_5, SiF_6^{2-}.

^{31}P NMR of HPF_2 (cases of $J_{P-H} > J_{P-F}$ and $J_{P-F} > J_{P-H}$), phosphorous acids, P_4S_3, cis and trans $[PtX_2(PPh_3)_2]$, fac and mer isomers of $Rh(PPh_3)_3Cl_3$, phosphazenes, Pincer phosphine compounds.

^{13}C NMR of carbonyl compounds. NMR of boron compounds,-Effect of quadrupolar nuclei on the ^1H NMR spectra.

Overview of ^{119}Sn (NMR spectra of organotin oxides and hydroxides) and ^{195}Pt NMR, Satellite spectra.

Study of fluxional behavior of molecules such as organometallic complexes of η^2-olefins, η^3-allyl and dienyl. NMR of paramagnetic molecules – isotropic shifts, contact and pseudo-contact shifts, Lanthanide shift reagents.

UNIT IV

4. EPR Spectroscopy

Theory of EPR spectroscopy, hyperfine splitting of CH_3, *p*-benzosemiquinone, bis(salycylaldimine)copper(II)complex, spin densitiy. McConnell relationship, g value and factors affecting the magnitude of g and A tensors in metal complexes, Zero-field splitting, Kramers degeneracy. Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – Applications of EPR to a few biological molecules containing Cu(II) and Fe(III) ions.

UNIT V

5. X-Ray Diffraction

Crystal as lattice concept-lattice and reciprocal lattice, Miller indices, stereographic projection, Equivalent positions and special positions, unit cell and asymmetric unit. Diffraction of X-rays- Bragg's condition, 32 crystal classes, 14 bravais lattice, seven crystal systems, screw axis and glide planes, symmetry elements and its graphic symbols. Laue Method, Bragg Method, Debye – Scherrer method of X ray structural analysis of crystals, space groups and its deduction from systematic absences, Phase problem in structure analysis. Atomic and crystal Structure factor calculation, Fourier synthesis, heavy atom method, refinement of structures. Overview on Crystallographic Information File (CIF).

UNIT VI (Not for final examination)

6. Mossbauer Spectroscopy

Theory-Doppler effect - isomer shift-quadruple splitting-magnetic hyperfine splitting-application of MB spectroscopy to inorganic compounds

Text and Reference Books

1. R.S. Drago, *Physical Methods in Inorganic Chemistry*; Affiliated East-West press Pvt. Ltd, New Delhi, 2012 (Units I-IV).
2. R.S.Drago, *Physical Methods for Chemist*;Saunders College Publication, Philadelphia, 1992.
3. F.A. Cotton and G.Wilkinson, *Advanced Inorganic Chemistry*, 6thEd., Wiley-Eastern Company, New Delhi 1999.
4. H. H. Willard, L. L. Merritt, J. A. Dean, F. A. Settle, *Instrumental Method of Analysis*, 7th Edn. CBS publishers 2011.
5. W-K. Li, G-D. Zhou, T. C. W. Mak, *IUCR Text on Crystallography: Advanced Structural Inorganic Chemistry*, Oxford University Press, 2008. (Unit V)
6. W. Clegg, *Crystal Structure Determination*, Oxford Chemistry Primers, Oxford University Press 1998. (Unit V)

7. Y. Waseda, E. Matsubara, K. Shinoda, *X-ray Diffraction Crystallography*, Springer, 2011. (Unit V)
8. B. D. Cullity and S. R. Stock, *Elements of X-ray Diffraction* Pearson 3rd Edn. 2014. (Unit V)

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Spectral characterization of inorganic compounds.
- Applications of electronic spectroscopy to various metal complexes.
- Energy level diagrams for d^1 to d^9 states.
- Applications of IR and Raman spectroscopy to single molecules.
- Concepts of multinuclear NMR spectroscopy.
- Application of EPR spectroscopy to inorganic complexes.
- Structural chemistry of molecules using X-ray diffraction.
- Stepwise structural elucidation of compounds using combined spectroscopic techniques.

SEMESTER-III **HOUR/WEEK: 6**

CHE533CC **CREDIT: 5**

PHYSICAL CHEMISTRY - III

OBJECTIVES

- Applications of quantum chemistry to chemical bonding
- To understand the basic concepts of statistical thermodynamics, polymer chemistry, electrochemistry, analytical chemistry and molecular spectroscopy

UNIT I

1. Applications of quantum Chemistry

Molecular Orbital and valence bond theory of molecules: The Born–Oppenheimer approximation, MO treatment of H_2^+– molecular term symbols –Hybridisation - solving wave functions for sp^1, sp^2&sp^3 hybrid orbitals - Delocalised systems: Huckel theory of conjugated systems like ethylene and butadiene – Schrodinger equation for rotational, vibrational and electronic components and their selection rules.

UNIT II

2. Statistical Thermodynamics

Combinatory rule - probability theorem - permutations and combinations - concept of ensembles energy states and energy levels - macro-states and micro-states - Maxwell-Boltzmann statistics - thermodynamic probability, Sterling's approximation, Legrange's undeterminedmultiplier, distribution functions.

Molar partition function - separation of partition function- translational, rotational, vibrational and electronic partition functions, combined partition function- equilibrium constant and partition function. Quantumstatistics - Bose-Einstein and Fermi-Dirac statistics - photon gas -degeneracy and Bose Einsteincondensation, application to liquid He - negative Kelvin temperature.

UNIT III

3. Polymer Chemistry

Overview of polymers - structure and classification of polymers - kinetics and mechanism of free radical and ionic polymerizations - degree of polymerization - condensation and coordination polymerizations - Zeigler-Natta polymerization - copolymerization - molecular weight of polymers- number and weight average molecular weights - determination of molecular weight – light scattering and viscosity methods - gel permeation chromatography.

UNIT IV

4. Electrochemistry-Electrodics

The electrical double layer - polarizable and non-polarizable interfaces - structure of electrical double layer - double layer models - Helmholtz, Guoy-Chapman and Stern models.

Kinetics of electrode processes - current-potential curve - Butler-Volmer relation and its approximations - symmetry factor and transfer coefficient - Tafel equation - charge transferresistance - Nernst equation from Butler-Volmer equation - primary and secondary batteries – fuelcells - corrosion and its prevention methods.

UNIT V

5. Data, chromatographic and thermal analysis: Mean and standard deviation; absolute and relative errors; linear regression; covariance and correlation coefficient.

Analytical Techniques: Principle and applications of adsorption, partition, ion exchange and solvent extraction – chromatographic methods – TLC, HPLC and GC. Applications of atomic, molecular and emission spectroscopy in quantitative analysis

Thermal analysis: TGA, DTA, DSC- Applications. Light scattering techniques including nepelometry

UNIT VI (Not for final examination)

6. Electronic spectroscopy of molecules

Born-Oppenheimer approximation, sequence and progression, term symbols, Frank-Condon principle, rotational fine structure, fortrat parabolae, predissociation, dissociation energies, Birge-Sponer extrapolation, oscillator strength, solvent effects, photoelectron spectroscopy.

Text Books

1. D.A. Mcquarrie, Quantum Chemistry, University Science Books, 1998
2. A.K. Chandra, Introductory Quantum Chemistry, 4thed,. Tata McGraw Hill, 2009.
3. P.W. Atkins,Physical Chemistry, 7th Ed., OxfordUniversity press, 2002.
4. D.A. McQuarrie and D. Simon, Physical chemistry, A Molecular Approach ,Viva Books Pvt. Ltd, 2003.
5. J. Rajaram and J.C. Kuriacose, Thermodynamics for Students of Chemistry – Classical, Statistical and Irreversible, ShobhanLalNagin, New Delhi, 1981.
6. S. Glasstone, Text book of Physical Chemistry, McMillan, 1974.
7. C.E. Carraher, Polymer chemistry, 6th Ed, Marcel Deckker, 2003.
8. F.W. Billmeyer, Jr., A Text Book of Polymer Science, John Wiley, 1971.
9. V.R. Gowariker, N.V. Viswanathan, J. Sreedhar, Polymer Science, New Age Publishers, 1986.
10. Instrumental Methods of Analysis, Sixth Edition (Willard, Hobart H.; Merritt, Lynne L,; Dean, John A,; Settle, Frank A., Jr.)
11. G. D. Christian, Analytical chemistry, 6th edition, 2004.
12. Skoog and West, Fundamentals of analytical chemistry, 4th edition.
13. Fritz and Schenk, Quantitative analytical chemistry, 5th edition.

Reference Books

1. F.L. Pillar Elementary Quantum Chemistry, McGraw Hill 1968
4. J.P. Lowe, K.A.Peterson, Quantum Chemistry, 3rd Ed, Elsevier, 2006.
5. I.N. Levine, Quantum Chemistry, 5th Ed, Prentice Hall, 2000.

6. P.W. Atkins, Molecular Quantum Mechanics,2nd Ed., OxfordUniv. Press, 1987.
7. J. Goodisman, Contemporary Quantum Chemistry, Planum Press, 1977.
8. R.K. Prasad, Quantum Chemistry,New Age International Publishers, 1997.
9. H. Metiu, Quantum Mechanics, Taylor & Francis, 2006.
10. D.A. McQuarrie, J.D. Simon, Molecular Thermodynamics, University Science Books, Sausalito, 1999.
11. F.W. Sears, Thermodynamics, Kinetic theory of Gases and Statistical Mechanics, 2nd Ed., Addition Wesley, 1972.
12. H. Metiu, Physical Chemistry, Thermodynamics Taylor & Francis, 2006.
13. P.J. Flory, Principles of Polymer Chemistry, CornellUniversity Press, 1971.
14. A. Tager, Physical Chemistry of Polymers, Mir Publishers, 1978.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Applications of quantum chemistry to chemical bonding.
- Basic concepts of statistical thermodynamics, partition function and quantum statistics.
- Overview of polymers and polymerization.
- Determination of molecular weight of polymers by various techniques.
- Fundamentals of electrochemistry.
- Different types of batteries and fuel cells.
- Impacts of corrosions and its prevention methods.
- Basic concepts of data and errors.
- Handling and applications of various chromatographic techniques.
- Applications of various thermal analyses.

SEMESTER-3 **HOURS/WEEK: 6**
CHE534CC **CREDITS: 5**

ADVANCED TOPICS IN CHEMISTRY -III

OBJECTIVES

- **To learn proton NMR spectroscopy**
- **To study carbon NMR & NQR spectroscopy**
- **To learn various electro-analytical techniques**
- **To understand, Microwave Spectroscopy and Infrared Spectroscopy**

Unit I

1. Proton NMR

^{1}H NMR Spectroscopy – Multiplicity – Coupling constant – First order and second order proton, Spin-spin splitting – Dependence of *J* on dihedral angle – Vicinal and geminal coupling constants – Karplus equation – Long range coupling constants – Influence of stereochemical factors on chemical shift of protons – Simplification of complex spectra – Double resonance techniques, shifts reagents – Chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOH, NH, NH_2), an elementary treatment of NOE phenomenon. (**To be expanded)**

Unit II

2. Carbon NMR

Organic: ^{13}C NMR Spectroscopy – Basic theory of FT–NMR, Relaxation – Broad band decoupling – Off resonance decoupling and chemical shifts of common functional groups – DEPT spectra – Identification of small compounds based on NMR data.

2D Techniques: ^{1}H-^{1}H COSY – ^{1}H-^{13}C COSY – HMBC and NOESY. (**To be expanded)**

UNIT III

3. NQR Spectroscopy

Characteristics of quadrupolar nucleus – Effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – Applications of NQR spectroscopy.

4. Mossbauer Spectroscopy

Isomer shifts – Magnetic interactions – Mossbauer emission spectroscopy – Applications to iron and tin compounds.

Unit IV

5. Electromagnetic radiation and Infrared Spectroscopy

Electromagnetic radiation - interaction of electromagnetic radiation with molecules - types of molecular spectroscopy - factors affecting line width and intensity - signal to noise ratio and resolving power - absorption and emission spectroscopy.

6.Infrared Spectroscopy: vibrating diatomic molecule - harmonic and anharmonic oscillators - diatomic vibrating rotator - vibrations of polyatomic molecules - molecular vibrations, types of molecular vibrations, rotational vibrational spectra of linear and symmetric top molecules.

Unit V

7.Microwave Spectroscopy - Rotation of molecules - rotational spectra of rigid rotator, intensities of rotational lines, effect of isotopic substitution - rotational spectrum of non-rigid rotator - linear & symmetric top molecules - Stark effect.
Applications of microwave spectroscopy - determination of bond length, bond angle dipole moment and atomic mass from microwave spectra.

8. Raman Spectroscopy:

Raman spectroscopy- classical and quantum theory of Raman effect- rotational Raman spectra- linear, symmetric top molecules-vibrational Raman spectra- Raman activity of vibrations, rule of mutual exclusion, polarizability ellipsoids- rotational Fine structures- Resonance Raman and Laser Raman spectroscopy.

UNIT VI (Not for final examination)

9. Electroanalytical methods

Amperometry-Principles and applications, amperometric titration with examples-comparison with other titration methods-Basic principles of electrogravimetry-Coulometry: principles- coulometry at controlled potential- coulometry at constant current-coulometric titrations-advantages and applications-Cyclic Voltammetry: Principles and simple analytical applications – Interpretation of cyclic voltammogram.

References and Text Books

1. R.S. Drago, *Physical Methods in Inorganic Chemistry*; Affiliated East-West press Pvt. Ltd, New Delhi, 2012 (for Units I, II, III & IV).
2. R. S. Drago, *Physical Methods for Chemistry,* Saunders College Publication, Philadelphia, 1992
3. C. N. Banwell, *Fundamentals of molecular spectroscopy,* Tata McGraw-Hill education, 1994.
4. D. C. Harris and M.D. Bertolucci, *Symmetry and spectroscopy*, 1978.

5. G. M. Barrow, *Introduction to molecular spectroscopy*, Mc-Graw-Hill international editions, 1962.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Basic concepts and applications of ^{1}H and ^{13}CNMR spectroscopy.
- Applications of NQR and Moss Bauer spectroscopy.
- Types of molecular spectroscopy.
- Principles and applications of IR and rotational spectroscopy.
- Various electro-analytical techniques
- Determination of bonding parameters and atomic mass by microwave spectroscopy.
- Principles and applications of Raman and Laser Raman spectroscopy.
- Difference between IR and Raman spectroscopy.

SEMESTER-IV **HOURS/WEEK: 6**
CHE541CC **CREDITS: 5**

ORGANIC CHEMISTRY – IV

OBJECTIVES

- To understand the basic concepts of retrosynthesis
- To study the natural products chemistry and its applications
- To study the amino acids, enzymes and vitamins

UNIT I

1. Synthetic Methodology

Introduction to disconnections – Synthons and Synthetic equivalents – Synthon approach – Electron donors (nucleophiles) – Electron acceptors (electrophiles) – Introduction of functional groups – Umpolung reactions – One group disconnections: alcohols, olefins, ketones, acids – Two group disconnections: 1,2-, 1,3-, 1,4- and 1,5-Difunctional compounds – Convergent Syntheses – Functional Group Interconversion – Functional Group Addition – Carbon-Heteroatom Bonds – Methods for 3- and 4-membered rings. Synthesis of mono- and difunctional open chain molecules – Mono and bicyclic molecules with substituents.

UNIT II

2. Natural Products Chemistry-Part A

Terpenoids: Introduction – Isoprene and special isoprene rules – Biosynthesis: Mevalonic acid pathway, Role of coenzymes, biosynthesis of Menthol, Camphor, Caryophyllene, Taxol skeleton and Squalene – Total Synthesis: Takasago synthesis of Menthol, Corey's synthesis of Caryophyllene (2008) and Longifolene, Curran's synthesis of Hirsutene and Pirrung's synthesis of Isocomene.

UNIT III

3. Natural Products Chemistry-Part B

Steroids: Introduction – Salient features of structural elucidation of cholesterol (synthesis not expected) – Stereochemistry of steroids – Biosynthesis of cholesterol – Reactions of steroids (a brief account) – Partial synthesis of Androsterone and Testosterone (from cholesterol) – Total synthesis: Johnson's synthesis of Progesterone and Vollhardt's synthesis of Estrone.

Prostaglandins: Nomenclature – Function – Total synthesis: Corey's synthesis of Prostaglandins $F_{2\alpha}$ and E_2.

UNIT IV

4. Natural Products Chemistry-Part C

Alkaloids: Introduction – Biosynthesis: Common reactions and mechanisms, Biosynthesis of Nicotine, Harmane, Camptothecin and Papaverine – Total Synthesis: Corey's synthesis of Epibatidine, Comin's asymmetric synthesis of Camptothecin and Woodward's synthesis of Reserpine.

Antibiotics: Penicillins, Cepholosporins, Streptomycin and Tetracyclines (only structures; not elucidation) – Total synthesis: Sheehan's synthesis of Penicillin V and Woodward's synthesis of Cepholosporin C.

UNIT V

5. Peptides, Enzymes, Biomimetic chemistry Nucleic acids, and Vitamins

Peptides: End group protecting group analysis of primary, secondary and tertiary structures – Peptides: Synthesis of di- and tri-peptides – Protection of N-terminal and C-terminal groups of proteins – solid phase peptide synthesis.

Enzymes: Basic aspects of enzymes and co-enzymes - B**iomimetic chemistry –** Non-covalent interactions and molecular recognition – Crown ethers – Cyclodextrins – Calixarenes as enzyme models.

Nucleic acids: Structures of RNA and DNA.

Vitamins: Introduction and functions of vitamins A_1 and A_2, Roche total synthesis of Vitamin H (Biotin).

UNIT VI (Not for final examination)

Biogenesis – The building blocks and construction mechanism of 1. Terpenoids – Mono, Sesqui, Di and Triterpenoids and cholesterol 2. Alkaloids derived from ornithine, lysine, nicotinic acid, tyrosine and tryptophan. 3. The shikimate pathway – cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavanoids and terpenoid quinones.

Text and Reference Books

I. I. L. Finar, Organic Chemistry, Vol.II, Pearson Education India; 5 Ed., 2002.
2. E.J. Corey, X-M. Cheng, The Logic of Chemical Synthesis, Wiley-Interscience; 1st Ed., 1995.
3. K.C. Nicolaou and E.J. Sorensen, Classics in Total Synthesis, Targets, Strategies, Methods, Wiley VCH, 1996.
4. S. Warren, P. Wyatt, Organic Synthesis: The Disconnection Approach, 2nd Ed., Wiley, 2008.
5. F.A. Carey and R.J. Sundberg, Advanced Organic Chemistry, Parts A & B, 5th Ed., Springer, 2007.
6. S.P. Stanforth, Natural product chemistry at a glance, Blackwell Publishing, 1st Ed., 2006.
8. Caryophyllene: *J. Am. Chem. Soc.* **2008**, *130*, 2954-2955; *Synfacts* **2008**, *8*, 0783.
9. Epibatidine: *J. Org. Chem.* **1993**, *58*, 5600-5602.
10. Camptothecin: *J. Am. Chem. Soc.* **1992**, *114*, 10971-10972.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Chemistry of natural products and its applications.
- Concepts of retrosynthesis.
- Total synthesis of natural products.
- Biosynthesis of different alkaloids.
- Structure, application and total synthesis of antibiotics.
- Concepts of biomolecules present inside the body.
- Important functions of peptides, enzymes and vitamins.
- Structure and functions of DNA and RNA.

SEMESTER-IV **HOURS/WEEK: 6**
CHE542CC **CREDITS: 5**

INORGANIC CHEMISTRY - IV
(Selected Topics in Inorganic Chemistry)

OBJECTIVES

- To understand the magnetic properties of complexes.
- To know the concepts on nuclear, inorganic photochemistry and solid state chemistry.
- To know the chemistry of lanthanides and actinides.

UNIT I

1. Magnetic Properties

Different types of magnetic behavior (dia, para, ferro and antiferromagnetism), mechanism of ferro and aniferromagnetic exchange pathways, magnetic moment and magnetic susceptibility-determination using NMR, Faraday and Guoy's Method, orbital contribution to a magnetic moment, spin canting and spin cross over compounds, single molecular magnets. Examples for bi, tri and tetranuclear coordination compounds with different spin system - calculation J in binuclear complex.

UNIT II

2. Nuclear Chemistry

Nuclear Reactions, Nuclear Cross section, Q value, types of reactions, transmutation, stripping and pick-up, spallation etc., fission, theories of fission, atom bomb, nuclear fusion, stellar energy, use of radio isotope in analytical chemistry, isotopic distribution analysis, neutron activation analysis, dating methods, applications of radio isotopes in agriculture industry and medicine.

UNIT III

3. Solid State Chemistry – I

Preparative methods: Solid state reactions, Chemical Precursor methods, co-precipitation, sol-gel metathesis, self-propagating high temperature synthesis, ion exchange reactions, intercalation/deintercalation reactions; hydrothermal and template synthesis, high pressure synthesis. Types of solid state reactions

UNIT IV

4. Solid State Chemistry – II

Defects in solids-stoichiometric and non-stoichiometric defects-dislocations, effects due to dislocations. Band theory of solids – metals and their properties, semiconductors – extrinsic (n and p type) and intrinsic, Hall effect, thermoelectric effects (Thomson, Peltier, Seeback); insulators-super conductivity, high temperature super conductor- Y-Ba-Cu super conductors (1-2-3 system)- general applications.

UNIT V

5. Chemistry of Lanthanides and Actinides

Lanthanides and actinides: electronic configuration-oxidation states, lanthanide contraction-effect of lanthanide contraction, magnetic and spectral properties of lanthanides. Some examples for coordination and organometallic compounds of lanthanides. Gd complexes as MRI agents and other applications of lanthanides compounds.

UNIT VI (Not for final examination)

6. Inorganic Photochemistry

Elementary ideas on the photosystems I and II - Photochemistry of Cr(III), Co(III) and Ru(II) - coordination compounds – photoaquation – photoanation – photoisomerisation – photo redox reactions – charge transfer photo chemistry – photosensitisation – solar energy conversiuon – photogalvanic cell – splitting of water to evolve hydrogen and oxygen – photochemistry of Pt(II) and Pt(IV) complexes.

Text and Reference books

1. R. Dutta, Syamal, *Elements of Magnetochemistry* East-West Press 2010. (Unit I)
2. H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Edn New Age International Publishers, 2011. (Unit II)
3. G. R. Choppin, J-O Liljenzin, J. Rydberg, C. Ekberg, *Radio Chemistry and Nuclear Chemistry* 2016. (Unit II)
4. A. R. West *Solid State Chemistry* and its Applications Wiley 2007 (Unit III and IV)
5. G. E. Rodgers, Inorganic and Solid State Chemistry Cengage Learning 2008 (Unit III and IV)
6. J.D. Lee, *Concise Inorganic Chemistry*, 5th Ed, Wiley, 2008 (Units III - V)
7. B. Sivashankar, *Inorganic Chemistry*, Pearson India Ltd. 2013. (All units)
8. A.W. Adamson, E.D. Fleishcer, Concepts in Inorganic photochemistry, 1963.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Different magnetic properties of metal complexes.
- Determination of magnetic susceptibility of metal complexes by different methods.
- Principles and applications of nuclear chemistry.
- Concepts of atom bomb and stellar energy.
- Applications of radio isotopes in agriculture industry and medicine.
- Basic concepts of solid state chemistry and inorganic photochemistry.
- Concepts of semiconductors, insulators and superconductors.
- Chemistry of lanthanides and actinides and their applications.

SEMESTER-IV **HOUR/WEEK: 6**
CHE543CC **CREDIT: 5**

PHYSICAL CHEMISTRY – IV

OBJECTIVES

- To understand the basic concepts of material chemistry and nanomaterials
- To learn the basics of Biophysical chemistry and biophysical techniques
- To understand the basic concepts of photochemistry methods and supramolecular chemistry

UNIT - I

1. General introduction to nanoscience

Forms of matter – crystalline and amorphous materials – surface tension (definition only) – surface energy – surface to volume ratio – surface relaxation – dimensionality and electron confinement - 0D, 1D and 2D nanostructures – size dependent properties – Mechanical properties, fracture toughness, Hall-Petch relation – superplasticity; Optical properties: absorption, surface plasmon absorption, photoluminescence; magnetic properties – hysterisis loop – superparamagnetism; electrical conductivity – electronic properties – applications of nanomaterials.

UNIT - II

2. Synthesis and characterization of nanomaterials

Top-down and bottom-up approaches – nanoparticles by homogeneous nucleation – nucleation process – size of the nuclei – influence of nucleation rate on the size of the crystal – growth processes – steric and electrostatic stabilizations – chemical methods – sol-gel techniques – kinetically confined synthesis of nanoparticles – template based synthesis: hard and soft template methods – sonochemical method – electrochemical method – particle size determination.

Principles, instrumentation and applications of SEM, TEM and AFM.

UNIT - III

3. Biophysical chemistry principles

Basic aspects of structure, classification and functions of carbohydrates, Nucleic acids, DNA and RNA conformations-Amino acids, polypeptides, proteins-primary, secondary, tertiary and quaternary structures-protein folding - molecular forces in folding- Ramachandran diagram-structure of phospholipids-Surface active molecules in biological systems: lecithin (phosphatidylcoline), cholesterol- vesicles- interaction between proteins and lipids- Proteins in biological catalysis, enzymes.

UNIT - IV

4. Biophysical Chemistry – Methods

Structural and conformational analysis of biomacromolecules– spectroscopic methods - NMR - fluorescence - FT-IR – Circular Dichroism - microscopic methods – Fluorescence and confocal Microscopy, Electron Microscopy - thermodynamics and kinetics of Biomolecular interactions - ITC - SPR – Q.

UNIT - V

5. Photochemistry methods

Absorption, CW photolysis, photoreactors, light Sources, filters, photochemical quantum yield and intensity measurements - detectors-PMT, Diode array, CCD, ICCD. Time resolved techniques – pump-probe methods and instrumentation: Lasers-nanosecond, picosecond and femtosecond.

UNIT VI (Not for final examination)

6. Supramolecular Chemistry

Introduction to Supramolecular Chemistry – definitions – concepts – molecular forces - covalent bonding, ion – ion, ion – dipole, dipole – dipole, hydrogen bonding, cation – π, π-π interactions, van der Waals forces, hydrophobic and solvent effects – Common motifs in Supramolecular Chemistry – Host/Guest Chemistry, cation, anion and neutral molecule binding. Molecular receptors and design principles. Cryptands, cyclophanes, calixarenes and cyclodextrins. Methods for binding constant measurement- Nucleic acid structure & molecular recognition - DNA & RNA, Protein – primary, Secondary, tertiary & Quaternary Structure – Protein folding problem – principles of molecular association and organization – SAMs, micelles, vesicles and cell membrane – Supramolecular reactivity and catalysis- Molecular devices and Nanotechnology.

Text and Reference books

1. Guozhong CaO, Nanostructures and Nanomaterials: Synthesis, Properties and Applications, Imperial College Press, 2004.
2. C.P.Poole, Jr., and F.J. Owens, Introduction to Nanotechnology, John Wiley & Sons, 2006.
3. G.L. Hornyak, J. Dutta, H.F.Tibbals, A.K. Rao, Introduction to Nanoscience, CRC Press, Taylor & Francis Group, 2008.
4. R.M.J. Cotterill, Biophysics-An introduction, John Wiley, 2004.

5. Van Holde K. E., Johnson W. C. and Ho P.S, Prentice.Principles of Physical Biochemistry -HallInternational. inc. First edition,1998. ISBN-0-13-649351-3.
6. Tinoco,Sauer, Wang and PuglisiPhysical Chemistry; Principles and Applications in Biological Sciences, Pearson Education, Fourth edition (2007).
7. Ira Blei and George Odian. General, Organic, and Biochemistry: Connecting Chemistry to Your Life, 2nd edition, 2006.
8. Proteins; Structures and Molecular Properties, Creighton E.T., W. H. Freeman and Company (New York) Second edition, 1993.
9. M.J. Jones, Biological Interfaces, Elsevier, 1975.
10. N.J. Turro Modern Molecular Photochemistry, University Science Books, 1991.
11. J.R. Lakowicz Principles of Fluorescence Spectroscopy,3rdedn Kluwer, 2006.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Basic concepts of materials chemistry.
- Properties and applications of nanomaterials.
- Synthesis and characterization of nanomaterials.
- Principles, instrumentation and applications of SEM, TEM and AFM.
- Principles of biophysical chemistry and biophysical techniques.
- Structure, classification and functions of carbohydrates, nucleic acids, proteins, polypeptides and amino acids.
- Structural and conformational analysis of bio-macromolecules.
- Basic concepts of photo chemistry methods and supramolecular chemistry.

ADD-ON COURSE CURRICULUM

SEMESTER-I **HOUR/WEEK: 6**
CHE511AC

MEDICINAL CHEMISTRY

OBJECTIVES

- **To learn about drugs, mechanism of action, design, development, Molecular modeling and Computer aided drug design**
- **Application and action mechanism of antibacterial, antiviral, anticancer and cardiovascular drugs**

Unit-I:

Introduction to Drugs

Definition – Sources and classification of drugs – Drug targets – Important terminologies in medicinal chemistry.

Unit-II:

Drug Action

Role of intermolecular forces in drug action – Pharmacokinetics and pharmacodynamics: administration, absorption, distribution, metabolism, elimination of drugs.

UNIT-III:

Drug Design and Development

Structure Activity Relationships – QSARs – Preclinical trials: pharmacology, toxicology, metabolism and stability studies – Clinical trials: phase I-IV studies – ethical issues.

UNIT-IV:

Antibacterial and Antiviral Drugs

Antibacterial agents – Mechanism of action – Antibacterial agents that act against cell metabolism (sulfonamides), inhibit cell wall synthesis (penicillins), impair protein synthesis (tetracyclines) and act on nucleic acids (fluoroquinolones) – Antiviral agents: Nucleic acid synthesis inhibitors and inhibitors of viral protein synthesis.

UNIT-V:

Anticancer and Cardiovascular Drugs

Anticancer drugs and their mechanism of action – Role of antimetabolites, enzyme inhibitors, antisense drugs, and interchelating agents in cancer chemotherapy – Cardiovascular drugs: antiarrhythemic and antihypertension drugs.

Text and reference books:

1) Wilson and Giswald's Textbook of Organic Medicinal and Pharmaceutical Chemistry by John Block and John M Beale (Eds), Lippincott Williams & Wilkins, 11th edition, **2003**.
2) Fundamentals of Medicinal Chemistry by Gareth Thomas, John Wiley & Sons: Chichester, **2003**.
3) Medicinal Chemistry: An Introduction by Gareth Thomas, Wiley-Interscience, 2nd edition, **2008**.
4) An introduction to Medicinal Chemistry by Graham L. Patric, Oxford University Press, USA, 3rd edition, **2005**.
5) The Organic Chemistry of Drug Design and Drug Action by Richard B. Silverman, Academic press, 2nd edition, **2004**.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Sources, classification of drugs, targets of drugs
- Important terminologies used in medicinal chemistry and drug industry
- Different action of drugs at targets
- Design and development of drugs, clinical trials and ethical issues
- Antibacterial drugs and its mechanism of action
- Antiviral agents, anti-cancer drugs and its mechanism of action
- Molecular modeling and Computer aided drug design
- Cardiovascular drugs and its mechanism of action

SEMESTER-II **HOUR/WEEK: 6**

CHE521AC

ENVIRONMENTAL CHEMISTRY

OBJECTIVES:

- **To understand environment oriented chemistry**
- **To learn about hydrosphere, aquatic pollution, water quality standards, purification and treatment of water**
- **To learn composition of soil and soil pollution**
- **To learn about atmosphere, air pollution and environmental toxicology**

Unit I

Environment: Introduction – Composition of atmosphere – Biogeochemical cycles of Carbon, Nitrogen, Phosphorous, Sulphur, Oxygen and Water.

Unit-II

Hydrosphere: Chemical composition of water bodies – lakes, streams, rivers and wet lands etc. Hydrological cycle. Aquatic pollution – inorganic, organic, pesticides, agricultural, industrial and sevag, detergents, oil spills and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, contents of chloride, sulphate, phosphate, nitrate and microorganisms. Water quality standards. Analytical methods for measuring BOD, DO, COD, F, oil, metals, (As, Cd, Cr, Hg, Pb, Se, etc), residual chloride and chlorine demand. Purification and treatment of water

Unit-III

Soil : Composition of soil-soil pollution-causes and effects-industrial wastes-urban wastes-agricultural practices-radioactive pollutants-control of soil pollution.

Unit -IV

Atmosphere: Chemical composition of atmosphere - Chemical and photochemical reactions in atmosphere, Oxides of N, C, S, O and their effect, pollution by chemicals, chlorofluorohydrocarbons. Green house effect, acid rain, air pollution controls and their chemistry.

Unit V

Environmental Toxicology: Chemical solution to environmental problems, biodegradability, principles of decomposition, better industrial processes. Bhopal gas tragedy, Chernobyl, Three mile island, Sewazo and Minamata disasters.

Unit VI

Industrial Pollution: Cement, sugar, distillery, drug paper and pulp, thermal power plants, nuclear power plants, metallurgy polymers drugs etc., radionuclide analysis, disposal of wastes and their management

Text and Reference Books

1. Environmental Chemistry, S.E. Manahan, Lewis publishers.
2. Environmental Chemistry, Sharma & Kaur, Krishna publishers
3. Environmental Chemistry, A.K. De, Wiley Eastern
4. Environmental Chemistry, S.M. Khopkar, Wiley Eastern
5. Environmental Chemistry, C. Baird, W.H. Freeman

LEARNING OUTCOMES

After the completion of this course, students will be able to

- Demonstrate knowledge of chemical and biochemical principles of fundamental environmental processes in air, water, and soil.
- Develop an understanding of chemicals and their effects on the environment.
- Composition of soil and atmosphere
- Different types of pollutions and their controls
- Understand green house effect and global warming
- Develop an understanding of some basic principles of chemistry and apply these principles to current environmental issues
- Acquire broad knowledge of the field of environmental toxicology and chemistry including basic principles, target organ toxicity and the toxicity of a select group of chemical compounds.
- Describe water purification and waste treatment processes and the practical chemistry involved.

SEMESTER-III **HOUR/WEEK: 6**

CHE531AC

MATERIALS CHEMISTRY

OBJECTIVES:

- **To understand the principles and applications of nanoscience and technology**
- **Chemicals and non-chemical approaches to material synthesis**
- **Emerging materials in chemistry**

Unit-I

Introduction to nanoscience and nanotechnology

Introducing ourselves to nano world- How nano materials behave-What is its importance in today's technology-Methods of synthesis of nanostructured materials.

Unit -II

Graphene

Fundamentals and applications - Introduction to graphene - Preparation and characterization graphene -Potential application of graphene

Unit -III

Chemical and non-chemical approaches to materials synthesis -Sol-gel science- Micro-emulsions- Microwave mediated synthesis of materials- solid-state synthesis- Hydrothermal and thermochemical methods

Unit-IV

Modern characterization of materials - DLS- Powder X – ray diffraction- SEM, TEM and AFM

Unit-V

Electrical, optical and magnetic properties of the materials and its measurements techniques -Energy materials- Batteries, photovoltaics and supercapacitors - Emerging materials chemistry

Text and Reference Books:

1. Materials science, J. C. Anderson, K. D. leaver and R. D. Rawlings, CRC press, 2003.
2. Magnetic nanoparticles, S. G. Gubin. Wiley-VCH.

3. Nanomaterials, B. Vishwanathan, Abe books.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Theoretical and practical knowledge related to modern materials chemistry and nanotechnology
- Principles and applications of nanoscience and technology
- Importance of nano-materials over macro materials
- Fundamentals and applications of graphene
- Chemicals and non-chemical approaches to material synthesis
- Different characterization techniques to materials
- Electrical and optical properties of materials
- Applications of emerging chemical materials

SEMESTER-IV **HOUR/WEEK: 6**

CHE541AC

Polymer Chemistry

OBJECTIVES

- **To learn fundamentals of polymer chemistry**
- **To learn Different types of polymerization**
- **To learn natural and synthetic polymers and characterization techniques**

Unit I:
Basics

Importance of polymers-Basic concepts-repeating units, degree of polymerisation-linear, branched and network. Polymerisation conditions and polymer reactions. Polymerization in homogeneous and heterogeneous systems.

Unit-II:
Methods of polymerisation

Bulk polymerisation, Solution polymerisation, Emulsion polymerisation, Suspension polymerisation and Interfacial polymerisation.

Unit-III:
Types of Polymerisation

Types of polymerisation-Free radical polymerisation, Generation of free radicals-Initiation, propogation and termination-Condensation polymerisation-Mechanisms. Copolymerisation-Types of copolymerisation-Mechanism-Block and graft copolymers.

Unit-IV:
Natural and Synthetic Polymers

Synthesis, properties and applications of plastics and elastomers. Natural rubber and other isoprene polymers, rubbers derived from butadiene-acrylic acid copolymers. Thermoplastics and thermosetting polymers-PVC, polyvinyl acetate (PVA), polyamides, Nylon-66, polyesters, phenolic resin and epoxy resins.

Unit –V:
Polymer Characterization

Polydispersion-molecular weight concept-Number, weight and viscosity average molecular weights- The practical significance of molecular weight- measurement of molecular weight by viscosity and ultracentrifugation methods-X-Ray diffraction study-Thermal analysis and physical testing tensile strength.

Books Suggested

1. Textbook of Polymer Science, F.W. Billmeyer Jr, Wiley.
2. Polymer Science, V.R. Goweriker, N.V. Viswanathan and J. Sreedhar, Wiley-Eastern.
3. Functional Monomers and Polymers, K. Takemoto, Y. Inaki and RM. Ottanbrite.
4. Contemporary Polymer Chemistry, H.R. Alcock and F.W. Lambe, Prentice Hall.
5. Physics and Chemistry of Polymers, J. M.G. Cowie, Blackie Academic and Professional.
6. Principles of polymer chemistry, P. J. Flory.

LEARNING OUTCOMES

After the completion of this course, students will be able to understand about

- Fundamentals of polymer chemistry
- Various types of polymerization methods
- Concepts of natural and synthetic polymers
- Thermoplastics and thermosetting plastics
- Preparation and applications of few polymer materials
- Determination of molecular weight of polymers by different methods
- Characterization techniques of polymers
- Uses of polymers used in daily life

Course Details

PART B

COURSES OFFERED BY CHEMISTRY DEPARTMENT TO THE STUDENTS OF OTHER DEPARTMENTS

Two elective papers, one each in second and third semester, are offered to two year M.Sc course students of other departments. Two papers one each in second and third semester, are also offered to Five Year Integrated M.Sc students of other departments.

SECOND SEMESTER

Elective papers offered to two year M Sc course students of other departments.

CHE526-1EC Selected Topics in Chemistry – I	25	75	100	4
Or				
CHE526-2EC Concepts and Models in Chemistry	25	75	100	4

Paper offered to M Sc - Five Year Integrated Physics, Geosciences, Life Sciences and Biomedical Sciences

Concepts and Models in chemistry	25	75	100	4

THIRD SEMESTER

Elective papers offered to two year M.Sc course students of other departments

CHE535-1EC Selected Topics in Chemistry – II	25	75	100	4
Or				
CHE535-2EC General Chemistry	25	75	100	4

Paper offered to M Sc - Five Year Integrated Physics

General Chemistry	25	75	100	4

SECOND SEMESTER

CHE526-1EC: SELECTED TOPICS IN CHEMISTRY - I

(EC offered to two M.Sc Students of other Departments in the second semester)

UNIT I

1. Introduction to Spectroscopy

Electromagnetic radiations and spectroscopy – UV-Visible spectroscopy: Theory – Beer-Lambert's law (derivation not required) – Important terminologies: molar absorptivity, chromophore, auxochrome, bathochromic shift, hypsochromic shift – Instrumentation (block diagram only) – Spectra of acetone and benzene – IR spectroscopy: Theory – Molecular vibrations – Characteristic group frequencies – Instrumentation (block diagram only) – Spectra of acetone and ethanol – NMR spectroscopy: Theory – Chemical shift – Spin-spin splitting – Instrumentation (block diagram only) – Spectra of ethanol and ethyl benzene – Mass spectroscopy: Introduction – Application for determination mass for simple organic molecules.

UNIT II

2. Amino acids and Proteins

Structure – Classification – Nomenclature – Functional groups – Isoelectric point – Peptide structure – Structural levels of proteins – Primary, secondary, tertiary and quaternary, alpha, beta helix – Collagen, fibrous and globular proteins – Nucleic acids: Structure of RNA and DNA.

3. Enzymes

Classification of enzymes – Basic aspects of enzymes – Factors affecting enzyme activity: pH, temperature, substrate concentration – Examples of Coenzymes and its function.

UNIT III

4. Ionic equilibria in aqueous solution

Acids and bases, Arhenius theory, Lowry-Bronsted Concept, Lewis concept – Self ionization of water – Weak acids and bases, dissociation constants – hydrolysis – buffer solutions, action of buffers – acid base indicators – Acid-base titrations – basics , Complex ion equlibria.

UNIT IV

5. Oxidation – Reduction reactions and redox potentials

Concept of Oxidation state (Oxidation number), rules to assign oxidation states in polyatomic molecule – Half-reaction concept – balancing oxidation – reductions by half – reaction method – Galvanic cells, various types of electrode – Standard electrode (cell) potential – various conventions regarding half cell potentials – Nernst equation – Chemical and concentration cells – cell potentials and equilibrium constants.

UNIT V

6. Metals in biology

Occurrence and availability of inorganic elements in organism – Biological function of inorganic elements – Biological ligands for metal ions – Coordination of proteins and enzymatic catalysis – Porphyrins and other macrocycles – Nucleobases, nucleotides and other nucleic acids as ligands – Metal ion transport and storage – Dioxygen transport – Oxygen transport and storage through hemoglobin and myoglobin – Alternative oxygen transport in some lower animals – Hemereythrin and hemocyanin

Text and Reference books:

Unit I and II

1. P.M. Silverstein, F.X. Wester, Spectroscopic Identification of Organic Compounds, 6th Ed., Wiley 1998.
2. J. Mohan, Organic Spectroscopy Principles and Applications, 2nd Ed., CRC, 2004.
3. W. Kemp, Organic Spectroscopy, 3rd Ed., MacMillon, 1994.
4. D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy, 3rd Ed., Brooks Cole, 2000.
5. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th Ed., Pearson, 1992.
6. I.L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS 1975.

Unit-III and IV

1. Bruce H. Mahan, University chemistry, Narosa Publishers, New Delhi, 1998.

Unit-V

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Purnima Publishing Company, New Delhi, 1997.
2. J. E. Huheey, Inorganic Chemistry, 3rd ed., Harper & Row Publishers, Singapore.
3. W. Kaim and B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York, USA.
4. G. L. Eichorn, Inorganic Biochemistry, Volumes 1 & 2, 2nd ed., Elsevier Scientific Publishing company, New York, 1973.

SECOND SEMESTER- CHE526-2EC: CONCEPTS AND MODELS IN CHEMISTRY

(EC Offered to two year M.Sc Students of Other Departments in the Second Semester)

UNIT I

1. Bio-organic Chemistry

Amino acids and proteins: Structure, classification, nomenclature and function of amino acids, functional groups, isoelectric point – Peptide structure, structural levels of proteins – primary, secondary, tertiary and quaternary, alpha, beta helix – collagen, fibrous and globular proteins.

Nucleic acids: Structures of RNA and DNA**.**

Enzymes: Co-enzymes – Classification – Characteristics, functions, factors affecting enzyme activity: pH, temperature, substrate concentration. Examples for coenzymes and its functions.

UNIT II

2. Metal Ions in Biology

Occurrence and availability of Inorganic elements in Organism - Biological function of inorganic elements - Biological ligands for metal ions – Coordination of Proteins and enzymatic catalysis – Porphyrins and other Macrocycles – Nucleobases, nucleotides and other Nucleic acids as ligands. Metal ion transport and storage – Cobalamines - Metals at the Center of Photosynthesis. Dioxygen transport: Oxygen Transport and Storage through Hemoglobin and Myoglobin. Alternative oxygen Transport in some Lower Animals: Hemereythrin and Hemocyanin.

3. Chemotherapy

Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action. Lithium in Pschycopharmacological drugs.

UNIT III

4. Chemical Bonding

Atomic structure – Core and valence electrons – periodicity – valence shells and chemical reactivity – valence and chemical formulas – covalent, ionic and co-ordinate bonds – hydrogen bonds – non-covalent interactions – electronic and molecular structure - σ, π and δ bonds – bond parameters – conformation, configuration – various representations – macromolecules and three dimensional structures.

UNIT IV

5. Chemical Thermodynamics

Energy and the First Law of Thermodynamics, Conservation of energy-principle, work and heat, enthalpy, exothermic and endothermic reactions, C_p & C_v, Hess's law of heat summation, use of standard enthalpies of formation – Entropy and the second law of Thermodynamics, Kelvin and Clausius statements of Second Law, definition of entropy, spontaneity and reversibility, entropy change of the system, molecular basis of entropy, free energy and chemical equilibrium, Factors affecting equilibrium.

UNIT V

6. Chemical Kinetics

Rate of Reaction, order of reaction - derivation of rate equation for first order reaction, Determination of rate equation by isolation method – Effect of temperature on reaction rate - Arrhenius equation - Enzyme Kinetics – Michaelis - Menten equation - Salt effect on reaction rate (derivation not needed).

Text and Reference books:

UNIT I

1. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th Ed., Pearson, 1992.
2. I.L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS 1975.

UNIT II

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Purnima Publishing Company, 1997.
2. J.E. Huheey, Inorganic Chemistry, 3rd. Ed., Harper & Row publisher, 1983.
3. W. Kaim and B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley

UNIT III

1. C.H. Snyder, The extra-ordinary chemistry of ordinary things, John Wiley, 1992.
2. B.H. Mahan, University chemistry, Narosa Publishers.

UNIT IV

1. Gordon M. Barrow, Physical Chemistry , Tata McGraw Hill, 1994.
2. Bruce H. Mahan, University chemistry, Narosa Publishers.

UNIT V

1. R. A. Alberty and R. J. Silbey, Physical Chemistry, Chapter 19, John Wiley, 1995.
2. P.W. Atkins, Physical Chemistry, ELBS and Oxford University Press, 1998.

SECOND SEMESTER- CONCEPTS AND MODELS IN CHEMISTRY

Paper offered to M.Sc - Five Year Integrated Physics, Geosciences, Life Sciences and Biomedical Sciences in Second Semester

UNIT I

1. Bio-organic Chemistry

Amino acids and proteins: Structure, classification, nomenclature and function of amino acids, functional groups, isoelectric point – Peptide structure, structural levels of proteins – primary, secondary, tertiary and quaternary, alpha, beta helix – collagen, fibrous and globular proteins.

Nucleic acids: Structures of RNA and DNA.

Enzymes: Co-enzymes – Classification – Characteristics, functions, factors affecting enzyme activity
pH, temperature, substrate concentration. Examples for coenzymes and its functions.

UNIT II

2. Metal Ions in Biology

Occurrence and availability of Inorganic elements in Organism - Biological function of inorganic elements - Biological ligands for metal ions – Coordination of Proteins and enzymatic catalysis – Porphyrins and other Macrocycles – Nucleobases, nucleotides and other Nucleic acids as ligands. Metal ion transport and storage – Cobalamines - Metals at the Center of Photosynthesis. Dioxygen transport: Oxygen Transport and Storage through Hemoglobin and Myoglobin. Alternative oxygen Transport in some Lower Animals: Hemereythrin and Hemocyanin.

3. Chemotherapy

Platinum complexes in Cancer therapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action. Lithium in Pschycopharmacological drugs.

UNIT III

4. Chemical Bonding

Atomic structure – Core and valence electrons – periodicity – valence shells and chemical reactivity – valence and chemical formulas – covalent, ionic and co-ordinate bonds – hydrogen bonds – non-covalent interactions – electronic and molecular

structure - σ, π and δ bonds – bond parameters – conformation, configuration – various representations – macromolecules and three dimensional structures.

UNIT IV

5. Chemical Thermodynamics

Energy and the First Law of Thermodynamics, Conservation of energy-principle, work and heat, enthalpy, exothermic and endothermic reactions, C_p & C_v, Hess's law of heat summation, use of standard enthalpies of formation – Entropy and the second law of Thermodynamics, Kelvin and Clausius statements of Second Law, definition of entropy, spontaneity and reversibility, entropy change of the system, molecular basis of entropy, free energy and chemical equilibrium, Factors affecting equilibrium.

UNIT V

6. Chemical Kinetics

Rate of Reaction, order of reaction - derivation of rate equation for first order reaction, Determination of rate equation by isolation method – Effect of temperature on reaction rate - Arrhenius equation - Enzyme Kinetics – Michaelis - Menten equation - Salt effect on reaction rate (derivation not needed).

Text and Reference books:

UNIT I

1. R.T. Morrison and R.N. Boyd, Organic Chemistry, 6th Ed., Pearson, 1992.
2. I.L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS 1975.

UNIT II

1. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Purnima Publishing Company, 1997.
2. J.E. Huheey, Inorganic Chemistry, 3rd. Ed., Harper & Row publisher, 1983.
3. W. Kaim and B. Schewederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley

UNIT III

1. C.H. Snyder, The extra-ordinary chemistry of ordinary things, John Wiley, 1992.
2. B.H. Mahan, University chemistry, Narosa Publishers.

UNIT IV

1. Gordon M. Barrow, Physical Chemistry , Tata McGraw Hill, 1994.
2. Bruce H. Mahan, University chemistry, Narosa Publishers.

UNIT V

1. R. A. Alberty and R. J. Silbey, Physical Chemistry, Chapter 19, John Wiley, 1995.
2. P.W. Atkins, Physical Chemistry, ELBS and Oxford University Press, 1998.

THIRD SEMESTER

CHE535-1 EC: SELECTED TOPICS IN CHEMISTRY - II

(EC offered to two years M.Sc Students of other Departments in the third semester)

UNIT I

1. Liquid Phase Chromatography on Columns: Stationary phase and eluents – Adsorption columns – Preparation of columns – Application of the sample – Types of elution – Simple and fractional elution – Flash chromatography – HPLC.

2. Gas Chromatography: Gas-Solid chromatography (GSC) – Gas-Liquid chromatography (GLC) – Scope of gas chromatography – Techniques and R_f values.

3. Thin Layer Chromatography: Outline of the method – Adsorbents – Mobile phase – Preparation of plates – Applications – Identification and R_f values – Preparative TLC – HPTLC.

UNIT II

4. Chemical thermodynamics: Definition: Systems, States and state functions-First law of thermodynamics – Hess' law and applications – Heat capacity – Reversibility and spontaneity – Second law of thermodynamics – Molecular interpretation of entropy – Third law of thermodynamics – Heat engines – Combustion heats – oxidation, heats of reactions – interconverstion of energy.

UNIT III

5. Chemical Bonding: Atomic structure – Core and valence electrons – periodicity – valence shells and chemical reactivity – valence and chemical formulas – covalent, ionic and co-ordinate bonds – hydrogen bonds – non-covalent interactions – electronic and molecular structure - σ, π and δ bonds – bond parameters – conformation, configuration – various representations – macromolecules and three dimensional structures.

UNIT-IV

6. Volumetric Analysis: Titration curves - Acid-base indicators – Applications of acid-base titration - Complexometric titrations – EDTA titrations and metal ion indicators – Precipitation titrations – Indicators for pricipitation titrations – Adsorption indicators - Applications.

7. Gravimetric Methods of Analysis: General principles – Stoichiometry – Formation and properties of precipitates – Applications of gravimetric analysis – Nickel estimation.

UNIT V

8. Pollution: Air pollution – types and sources, atmospheric chemistry, depletion of stratospheric ozone, industrial and transport-related air pollution, acid rain, green house effect- global warming and its effects. - Water pollution – types and sources, physical and chemical water pollutants, waste water treatment, criteria of water quality.

Text and Reference Books:

UNIT I

1. J. Sherma, B. Fried, Practical Thin-Layer Chromatography: A Multidisciplinary Approach, 1st Ed., CRC Press Inc. 1996.
2. J. Sherma, B. Fried, Handbook of Thin-Layer Chromatography, 3rd Ed., CRC Press Inc. 2003.
3. A.I. Vogel, A.R. Tatchell, B.S. Furnis, A.J. Hannaford, P.W.G. Smith, Vogel's Textbook of Practical Organic Chemistry, 5th Ed., Prentice Hall, 1996.

UNIT II

1. B.H. Mahan, University chemistry, Narosa Publishers, 1998.

UNIT III

1. C.H. Snyder, The extra-ordinary chemistry of ordinary things, John Wiley, New York, 1992.
2. B.H. Mahan, University chemistry, Narosa Publishers, New Delhi, 1998.

UNIT IV

1. V.V. Ramanujam, Inorganic Semi Micro Quantitative analysis
2. A.I. Vogel, Text Book of Quantitative Inorganic Analysis, 3rd Ed., Longman, 1966.

UNIT V

1. A.K. De, Environmental Chemistry 4th Ed., New Age International Limited, 2006.
2. B.K. Sharma, Environmental Chemistry, Goel Publishing House, India.

THIRD SEMESTER- CHE535-2EC: GENERAL CHEMISTRY

(EC Offered to two year M.Sc Students of Other Departments in the Third Semester)

UNIT I

Reactive Intermediates, Spectroscopy and Stereochemistry of Organic Compounds: Formation and Breaking of Bonds: Homolytic and Hetrolytic fission. Reactive intermediates:Carbocationns, Free radicals – Definition and simple example only. Introduction to Infra Red, Nuclear Magnetic Resonance (^{1}H and ^{13}C) spectroscopy application to organic compounds (Elementary aspects only)

Stereochemistry: Chirality, Biological signification of chirality (Natural chirality, Chiral drugs) configuration and conformation, R and S configuration, Optical activity, Enantiomers and Diastereomer, Resolution, separation of enantiomers.

UNIT II

Hetrocycles: Nomenclature, Furan, Thiophene, pyrole, pyridine, preparation and properties and uses.

Alkaloids: Definition of alkaloid, Extraction, general properties determination of chemical constitution of alkaloids, Classification, Ephdrine, Adrenaline, Nicotine only.

Terpenes: Classification occurrence, general properties, Extraction, structure determination and property Citral and Menthol only.

UNIT III

Catalysis: Different between Homogeneous and heterogeneous catalysis – Steady – state approach – enzyme Catalysis – Michaelis – Menten kinetics – Effect of p^{H} on enzyme catalyzed reactions.

Macromolecules: Classification of polymers – Molecular weights of polymers: Number average and weight average of polymers – Molecular weight determination by viscosity method.

UNIT IV

Fundamentals of Spectroscopy and Photochemistry: Absorption and emission of radiation – region of electromagnetic spectrum – line with, Intensity – Beer Lamborts law and applications. Various photochemical processes, Jablonski diagram – Fluorescence and Phosphorescence - Laser and applications.

UNIT V

High – Temperature superconductors: 1-2-3 compounds, Meissner effect, applications of superconductors. Catenation and heterocatenation. (SN)x as one dimensional conductor, two specific examples for inorganic rings and cages. Binuclear metal clusters. An example for metal cluster in biology.

UNIT VI

Metal ions in medicine and biology: An overview of metal ions in medicine and biology. Blue copper proteins – Plastocyanin as a typical example. Zinc metalloenzymes – structure and function of carboxypeptidase. Vitamin B_{12} – structure and any two specific reactions of B_{12} coenzymes. Metal based drugs – cisplatin as anticancer drug, mechanism of action. Inhibitors of metalloenzymes as drugs – allopurinol, antabase. Detoxification of metals by chelation therapy with respect to iron, aluminium, Copper, mercury, arsenic and cadmium.

Text and Reference Books:

UNIT I & II

1. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.
2. R.T. Morrison, R.N. Boyd, Organic Chemistry, 6th Ed., Prentice Hall, 2004.
3. I.L. Finar, Organic Chemistry, Vol.I & II, 5th Ed., ELBS 1975.
4. B.S. Bhal, A. Bhal, Text Book of Organic Chemistry, 14th Ed., S Chand and Co., 1997.

UNIT III & IV

1. R.A. Alberty and R.J. Silbey, Physical Chemistry, Jhon wiley & Sons, 1995.
2. P.W. Atkins, Physical Chemistry, Oxford University Press, 1998.
3. G.M. Barrow, Physical Chemistry, Tata McGraw Hill, 1994.

UNIT V & VI

1. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry, 4th Ed., Pearson Education, 2002.

THIRD SEMESTER-GENERAL CHEMISTRY
(Paper Offered to M.Sc Five Year Integrated Physics in Third Semester)

UNIT I

Reactive Intermediates, Spectroscopy and Stereochemistry of Organic Compounds: Formation and Breaking of Bonds: Homolytic and Hetrolytic fission. Reactive intermediates: Carbocations, Free radicals – Definition and simple example only. Introduction to Infra Red, Nuclear Magnetic Resonance (^{1}H and ^{13}C) spectroscopy application to organic compounds (Elementary aspects only)

Stereochemistry: Chirality, Biological signification of chirality (Natural chirality, Chiral drugs) configuration and conformation, R and S configuration, Optical activity, Enantiomers and Diastereomer, Resolution, separation of enantiomers.

UNIT II

Hetrocycles: Nomenclature, Furan, Thiophene, pyrole, pyridine, preparation and properties and uses.

Alkaloids: Definition of alkaloid, Extraction, general properties determination of chemical constitution of alkaloids, Classification, Ephdrine, Adrenaline, Nicotine only.

Terpenes: Classification occurrence, general properties, Extraction, structure determination and property Citral and Menthol only.

UNIT III

Catalysis: Different between Homogeneous and heterogeneous catalysis – Steady – state approach – enzyme catalysis – Michaelis – Menten kinetics – Effect of p^{H} on enzyme catalyzed reactions.

Macromolecules: Classification of polymers – Molecular weights of polymers: Number average and weight average of polymers – Molecular weight determination by viscosity method.

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High – Temperature superconductors: 1-2-3 compounds, Meissner effect, applications of superconductors. Catenation and heterocatenation. (SN)x as one dimensional conductor, two specific examples for inorganic rings and cages. Binuclear metal clusters. An example for metal cluster in biology.

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Metal ions in medicine and biology: An overview of metal ions in medicine and biology. Blue copper proteins – Plastocyanin as a typical example. Zinc metalloenzymes – structure and function of carboxypeptidase. Vitamin B_{12} – structure and any two specific reactions of B_{12} coenzymes. Metal based drugs – cisplatin as anticancer drug, mechanism of action. Inhibitors of metalloenzymes as drugs – allopurinol, antabase. Detoxification of metals by chelation therapy with respect to iron, aluminium, Copper, mercury, arsenic and cadmium.

Text and Reference Books:

UNIT I & II

1. J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.
2. R.T. Morrison, R.N. Boyd, Organic Chemistry, 6th Ed., Prentice Hall, 2004.
3. I.L. Finar, Organic Chemistry, Vol.I & II, 5th Ed., ELBS 1975.
4. B.S. Bhal, A. Bhal, Text Book of Organic Chemistry, 14th Ed., S Chand and Co., 1997.

UNIT III & IV

1. R.A. Alberty and R.J. Silbey, Physical Chemistry, Jhon wiley & Sons, 1995.
2. P.W. Atkins, Physical Chemistry, Oxford University Press, 1998.
3. G.M. Barrow, Physical Chemistry, Tata McGraw Hill, 1994.

UNIT V & VI

1. J.E. Huheey, E.A. Keiter, R.L. Keiter, Inorganic Chemistry, 4th Ed., Pearson Education, 2002.

CONCEPTS AND MODELS IN CHEMISTRY
(M.TECH 6 YEARS COURSE FOR BIOTECHNOLOGY, BIOINFORMATICS GEOINFORMATICS AND COMPUTERSCIENCES - I SEMESTER)

Credits: 4

UNIT I

1. Stereochemistry of Organic Compounds

Fundamentals of Organic Stereochemistry: Chirality – Optical activity – Configuration – Fischer projections – Elements of symmetry – Absolute configuration – Cahn-Ingold-Prelog rules of nomenclature – Enantiomers and diastereomers – Resolution of racemic mixture. Geometric Isomerism; E and Z system of nomenclature – Geometrical isomerism in cyclic compounds – Conformational Isomerism.

UNIT II

2. Introduction to Spectroscopy

Electromagnetic radiations, Theory and instrumentation of Ultraviolet-Visible, Infrared, Nuclear Magnetic Resonance, Mass spectroscopic techniques - Structure determination of simple organic compounds (Only basic aspects).

UNIT III

3. Nature of Chemical Bond

Valence Shell Electron Pair Repulsion Theory (VSEPR) – Valence Bond Theory (VBT) – Molecular Orbital Theory (MOT) – Small molecules like $BeCl_2$, BCl_3 , NH_3, H_2O - Inter halogen compounds (ClF_3, BrF_3, BrF_5, IF_5, IF_7).

4. Coordination Compounds

Types of ligands - Valence Bond Theory (VBT) – Coordination Geometries.

UNIT IV

5. Metal Ions in Biology

Occurrence and availability of Inorganic elements in Organism - Biological function of inorganic elements - Biological ligands for metal ions – Coordination of Proteins and enzymatic catalysis – Porphyrins and other Macrocycles – Nucleobases, nucleotides and other Nucleic acids as ligands. Metal ion transport and storage – Cobalamines - Metals at the Center of Photosynthesis. Dioxygen transport: Oxygen Transport and Storage through Hemoglobin and Myoglobin. Alternative oxygen Transport in some Lower Animals: Hemereythrin and Hemocyanin.

UNIT V

6. Chemical Thermodynamics

Thermodynamic terms – definition of system – open, closed, isolated – surroundings, properties of system - state of a system - thermodynamic equilibrium – isothermal, isobaric, isochoric and adiabatic processes - internal energy – mathematical form of first law, enthalpy – statement of second law of thermodynamics – definition of entropy – entropy change for a reversible process - entropy change for an isothermal expansion of an ideal gas - entropy of phase transitions – definition of free energy and work function – Gibbs Helmholtz equation.

UNIT VI

7. Chemical Kinetics

Kinetics of second order reaction – characteristics of second order reactions – half life period – examples of second order reactions – hydrolysis of ester by sodium hydroxide – simple problems in second order kinetics – kinetics of opposing, parallel and consecutive reactions – radioactive decay of polonium – effect of temperature on reaction rate – Theory of absolute reaction rate – steady – state principle.

Text and Reference Books

1. R.T. Morrison, R.N. Boyd, Organic Chemistry, 6th Ed., Pearson, 1992.
2. J. Mohan, Organic Spectroscopy Principles and Applications, 2nd Ed., CRC, 2004.
3. M. Senapati, Advanced Engineering Chemistry, 2nd Ed., Infinity Science, 2007.
4. J.D. Lee, Concise Inorganic Chemistry, 5th Ed, Wiley, 1999.
5. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, 4th Ed., John Wiley & Sons, 1986.
6. P.W. Atkins,Physical Chemistry, 7th Edn, Oxford University Press, 2002.
7. D. A. Mc Quarrie and D. Simon, Physical chemistry, A Molecular Approach, Viva Books Pvt. Ltd, 2003.
8. H. Metiu, Physical Chemistry, Kinetics, Taylor & Francis, 2006.
9. K.J. Laidler, Chemical Kinetics, 2nd Ed., Tata McGraw Hill, 1975.

CHEMISTRY PRACTICALS
for

M.TECH 6 YEARS COURSE FOR BIOTECHNOLOGY, BIOINFORMATICS GEOINFORMATICS AND COMPUTERSCIENCES - I SEMESTER

Credit : 1

1. Hydrolysis: Preparation of Salicylic acid from Methyl-salicylate
2. Benzoylation: Preparation of Benzanilide from Aniline
3. Oxidation: Preparation of Benzoic acid from Benzyl alcohol
4. Preparation of Tris(thiourea)copper(II) sulphate
5. Estimation of Ca^{2+} by EDTA titration
6. Determination of total hardness of a sample of hard water
7. Determination of distribution coefficient of Iodine between CCl_4 and water
8. Study of phase diagram of simple entectic system (Naphthalene-biphenyl)
9. Determination of rate constant of the acid catalysed hydrolysis of ester.

References

1. Vogel's Text Book of Practical Organic Chemistry, Pearson Education, 5th Ed. 2004
2. Vogel's Quantitative Inorganic Analysis
3. Findlay's Practical Physical Chemistry, Revised and edited by B.P. Levitt, 9th Ed, Logman, London,1985.

I YEAR – II SEMESTER
GENERAL CHEMISTRY
2010-11 ONWARDS

UNIT 1

Bonding concepts: Ionic, covalent, coordinate, metallic, hydrogen bonds and noncovalent bonds.

Hybridisation and geometry of molecules: methane, ethylene, acetylene and benzene. Homolytic and hetrocyclic fission of bonds – reactive intermediates – carbocations and free radicals

Heterocycles: Preparation, properties and uses of furan, thiopene, pyrrole and pyridine. Heterocycles present in RNA & DNA.

UNIT II

Stereochemistry: Stereoisomerism – Definition and classification. Optical isomerism-chirality, chiral achiral, symmetric, asymmetric molecules. Enatiomers, diasteromers, racemate, racemisation, resolution -specific rotation – meaning of (+) and (-) and d or 1 notations- lactic acid and tartaric acid-D& L configuration as applied to carbohydrates and amino acids – R-S configuration as applied to carbohydrates and amino acids – R-S configuration. Conformation – definition – conformationl structure of ethane, cyclohexane, glucose and fructose.

UNIT III

Coordination chemistry and bioinorganic chemistry: Definition with examples of ligand, types- coordination number – coordination sphere – coordination compounds chelation-chelates. Bio- coordination compounds – haemoglobin, chlorophyII, metal based drugs-cis-platin as anti-cancer drug- detoxification of metals by chelation therapy with respect to iron, aluminium, copper, mercury, arsenic and cadmium.

UNIT IV

Chemical kineties: Rate and order of a reaction-deter mination of order of a reaction (Ostwald's isolation method), Homogeneous catalysis – basic aspects.

Chemical thermody namies: Laws of thermodynamics, energy, entropy, free energy concepts.

Chemicl equilibrium: Reversible and irreversible reactions- equilibrium constant and relationship between Kc & Kp- Lechatelier's principle nad effects of change of concentration, temperature and pressure.

UNIT V

Solutions: Solution- definition-types –concentration of solutions (Molarity, Molality, Normality and Mole-fraction). Eledctrolytes- Weak and strong electrolytes-Ostwald's dilution law-Lewis and Bronsted concepts of acids and bases. Ionic product of water-

pH of solutions-pH scale –buffer solutions – importance of pH and buffer in biological systems.

Reference Books:

1. B.S. Bahl and A.Bahl, "Advanced Organic Chemistry". S.Chand & Company Ltd.
2. P.L. Soni and M.Katyal, "Text book of Inorganic Chemistry", Sultan Chand & Sons.
3. B.R. Puri, L.R.Sharma and M.S.Pathania, "Principles of Physical Chemistry", Vishal Publishing Co.,

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M. Tech. (6 year integrated course)

Engineering Chemistry

UNIT – 1: Chemical Bonding (9 h)

Electronic theory of valency – ionic, covalent, coordinate and metallic bonds – hydrogen bond and van der Waals forces – hybridization – VSEPR model and molecular shapes – molecular orbital (MO) theory – MO treatment of diatomic molecules.

UNIT-II: Chemical Thermodynamics (9 h)

Thermodynamic terms – definition of system – open, closed, isolated – surroundings, properties of system – state of a system – thermodynamic equilibrium – isothermal, isobaric, isochoric and adiabatic processes – internal energy – mathematical form of first law – enthalpy – statement of second law of thermodynamics – definition of entropy – entropy change for a reversible process – entropy change for an isothermal expansion of an ideal gas – entropy of phase transitions – definition of free energy and work – function – Gibbs – Helmholtz equation.

UNIT – III: Electrochemistry (9 h)

Redox reactions – concept of oxidation number – electrochemical cells: chemical and concentration cells – electrode potential – Nernst equation – standard electrodes: hydrogen , calomel and glass electrodes – reference electrodes – electrochemical series – measurement of pH – basic concepts of batteries and fuel cells – simple exaples.

UNIT-IV: Polymers (9 h)

Introduction – Nomenclature – Classification – Types of polymerization: addition, condensation and co-polymerisation – Mechanism of addition polymerization: free – radical, cationic and anionic mechanisms and co-ordination (Zeigler - Natta) polymerization – Preparation, properties and uses of some important polymers: polyethylene, PVC, polystyrene, polymethyl methacrylate, Teflon, polycarbonates, polyurethanes, polyethylene terephthalate, epoxy resins, nylon and bakelite – conducting polymers- examples.

UNIT – V: Spectroscopy (9 h)

Electromagnetic radiations and spectroscopy – UV – Visible spectroscopy: theory – Beer –Lambert's law (derivation not required)- important terminologies: molar absorptivity, chromophore, auxochrome, bathochormic shift, hypsochromic shift – instrumentation (block diagram only), spectra of acetone and benzene – IR spectroscopy: theory- molecular vibrations-characteristic group frequencies-instrumentation (block diagram only)-spectra of acetone and ethanol –NMR

spectroscopy: theory-chemical shift-spin-splitting-instrumentation (block diagram only)- spectra of ethanol and ethyl benzene

Text-Book:

P.C.Jain and M.Jain, "Engineering Chemistry", 15th Edition, Dhanpat Rai Publishing Company (P) Ltd,, New Delhi, **2007.**

Reference Books:

1. R.D.Madan, "Modern Inorganic Chemistry", S.Chand & Company Ltd,
2. B.R.Puri, L.R.Sharma and M.S.Pathania, "Principles of Physical Chemistry". Vishal Publishing Co.,
3. B.S.Bahl and A.Bahl, "Advanced Organic Chemistry", S.Chand & Company Ltd.

CHEMISTRY LAB

1. Estimation of hardness of water by EDTA method
2. Estimation of chloride in water by argentometry
3. Conductometric titration of strong acid vs. strong base
4. Conductometric determination of solubility of a sparingly soluble salt

5. Preparation of dibenzalpropanone (base-catalyzed aldol condensation)
6. Determination of molecular weight of polymers by viscometry

A minimum of five experiments should be offered.