KANNUR UNIVERSITY

(Abstract)

New Generation Course in affiliated Colleges-M.Sc. Chemistry with Drug Chemistry Specialization programme under credit based semester system- Scheme, Syllabus and model question papers of core and generic elective courses with modified Course Code- Implemented w.e.f 2020-21 admission-Orders issued

ACADEMIC C SECTION

Acad/C2/16581/NGC/2021 Dated: 18.10.2021

Read:-1. U.O No Acad/C2/16581/NGC/2021 dated 25.01.2021
2. U.O Note No. EX/EG-1-1/21498/PG/Oct2020 dated 14.09.2021
3. Letter No, Acad C2/2408/2020 dated 24.09.2021
4. Minutes of the meeting of Board of Studies in Chemistry (PG) held on 28.09.2021
5. Order of the Vice Chancellor dated 09.10.2021

ORDER

1. As per paper read (1) above, Scheme, Syllabus and model question papers of Core & Generic Elective Course of New Generation Programme M.Sc. Chemistry with Drug Chemistry Specialization under CBSS was implemented.
2. Examination Branch, as per paper read (2) above, pointed out the practical difficulty in conducting examinations for the new generation programme M.Sc. Chemistry with Drug Chemistry Specialization, as its Course Code is same as that of the conventional PG programme, M.Sc. Chemistry.
3. As per paper read (3) above, the Board of Studies in Chemistry (PG) was entrusted to modify the Course Code of the M.Sc. Chemistry with Drug Chemistry Specialization programm (CBSS).
4. The Board of Studies in Chemistry (PG), resolved to change the Course Code of M.Sc. Chemistry with Drug Chemistry Specialization programme by replacing the prefix CHE with CHD and Course Code of the Elective papers as CHD2E.01, CHD2E.02, CHD3E.03, CHD3E.04, CHD4E.05, CHD4E.06 respectively. As per paper read (4) the Chairperson of Board of Studies Chemistry (PG) submitted the Syllabus of M.Sc. Chemistry with Drug Chemistry Specialization programme after effecting the modification of courses codes.
5. The Vice Chancellor, after considering the matter in detail and in exercise of the powers of Academic Council conferred under Section 11(1) Chapter III of Kannur University Act 1996, accorded sanction to implement the modified Scheme, Syllabus and model question paper of Core Course and Generic Elective Course of M.Sc. Chemistry with Drug Chemistry Specialization offered at KMM Govt Women's College, Kannur, with effect from 2020-21 admission, subject to reporting to the Academic Council.
6. The modified Scheme, Syllabus and model question paper of Core Course and Generic Elective Course of M.Sc. Chemistry with Drug Chemistry Specialization programme are uploaded in the University website (www.kannuruniversity.ac.in).
7. The U. O read (1) above stands modified to this extent.

Orders are issued accordingly.

sd/-
BALACHANDRAN V K
DEPUTY REGISTRAR (ACAD)
For REGISTRAR

To: The Principal
KMM Govt Women's College, Kannur

Copy To: 1. The Examination Branch (through PA to CE)
2. PS to VC/PA to PVC/PA to Registrar
3. DR/ARI Academic
4. The Web Manager (for uploading in the website)
5. SF/DF/FC

KANNUR UNIVERSITY CIVIL STATION P.O. KANNUR Pin-670 002 THAVAKKARA

Forwarded / By Order

SECTION OFFICER

SYLLABUS

M Sc Chemistry with Drug Chemistry Specialization

Kannur University

M Sc CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION

(Syllabus under credit based semester system with effect from 2020 admission)

Master of Science in Chemistry is the Post Graduate level course aims at an advanced level understanding of major concepts, theoretical principles, experimental aspects and research aptitudes in chemical sciences. The syllabi of MSc programmes in chemistry offered in the affiliated colleges of the university under semester system was revised in the light of the decision of the Board of studies meeting in chemistry (PG) and the revised syllabi were effective from 2014 admission onwards. There were two independent PG programmes in chemistry, namely MSc Chemistry and MSc Material Chemistry and as per GO(Ms) No. 389/2020/HEDN dated 05/11/2020 a new PG programme in Chemistry with title M Sc CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION was sanctioned at KMM Govt. Women's College, Kannur. As per order no. Acad/C2/2408/2020 dated 27/11/2020, Kannur University have constituted the expert committee for framing regulations, curriculum and syllabus for this programme. The expert committee has prepared the curriculum and syllabus in accordance with the 2014 regulations in such a manner that M Sc CHEMISTRY WITH DRUG CHEMISTRY SPECIALIZATION is equivalent with the existing MSc programmes in Chemistry for employment and higher studies. All of these three PG programmes shall extend over a period of two academic years comprising of four semesters, each of 450 hours in 18 weeks duration.

Candidate with bachelor's degree in chemistry with Mathematics and Physics as subsidiary subjects are eligible for admission to these courses. Rules regarding minimum marks required for the bachelor's degree, reservation etc., will be as that laid down by the University from time to time. The course work shall be in accordance with the scheme of valuation and syllabus prescribed. All theory papers for M Sc Chemistry with Drug Chemistry specialization, except elective papers will be the same as that for M Sc Chemistry programme of affiliated colleges of the university. The course consists of four theory papers and three practical papers (to be continued in semester II) in the 1^{st} semester, three theory papers, one elective paper and three practical papers in the II^{nd} semester, three theory papers, one elective paper and three practical papers (to be continued in semester IV) in the III^{rd} semester. Two theory papers, one elective paper, three practical papers, a project and general viva voce in the IV^{th} semester. The students may select one elective paper from each of the elective group. Each theory paper and elective paper is of 3 hours duration and each practical paper is of 6 hours duration. The total marks for the entire course shall be 1500 and total credit for the entire course shall be 80. 20% of marks shall be allocated for internal assessment of theory and practical papers each.

1. The syllabus and scheme of examination is given below*.

COURSE STRUCTURE

Semester	Paper Code	Title	Hrs /wk	Exam Duration	Marks for ESA	Marks for CA	Total	Credit
I	CHD1C.01	Theoretical Chemistry - I	4	3	60	15	75	4
	CHD1C.02	Inorganic Chemistry - I	4	3	60	15	75	4
	CHD1C.03	Organic Chemistry - I	4	3	60	15	75	4
	CHD1C.04	Physical Chemistry - I	4	3	60	15	75	4
	CHD1P.01	Inorganic Chemistry Practical - I	3	Carried over to semester - II				
	CHD1P.02	Organic Chemistry Practical - I	3	Carried over to semester - II				
	CHD1P.03	Physical Chemistry Practical - I	3	Carried over to semester - II				
		Total :	25		240	60	300	16
II	CHD2E.01/ CHD2E.02	Elective Paper I*	4	3	60	15	75	4
	CHD2C.05	Theoretical Chemistry - II	4	3	60	15	75	4
	CHD2C.06	Organic Chemistry - II	4	3	60	15	75	4
	CHD2C.07	Physical Chemistry - II	4	3	60	15	75	4
	CHD1&2P. 01	Inorganic Chemistry Practical - I	3	6	40	10	50	2
	CHD1&2P. 02	Organic Chemistry Practical - I	3	6	40	10	50	2
	CHD1&2P. 03	Physical Chemistry Practical - I	3	6	40	10	50	2
		Total :	25		360	90	450	22
III	CHD3E.03/ CHD3E.04	Elective Paper II*	4	3	60	15	75	4
	CHD3C.08	Inorganic Chemistry - II	4	3	60	15	75	4
	CHD3C.09	Organic Chemistry - III	4	3	60	15	75	4
	CHD3C.10	Physical Chemistry - III	4	3	60	15	75	4
	CHD3P.04	Inorganic Chemistry Practical - II	3	Carried over to semester - IV				
	CHD3P.05	Organic Chemistry Practical - II	3	Carried over to semester - IV				
	CHD3P.06	Physical Chemistry Practical - II	3	Carried over to semester - IV				
		Total :	25		240	60	300	16
IV	CHD4E.05/ CHD4E.06	Elective Paper III*	4	3	60	15	75	4
	CHD4C.11	Inorganic Chemistry III	4	3	60	15	75	4
	CHD4C.12	Inter disciplinary topics and instrumentation techniques	4	3	60	15	75	4
	CHD3&4P. 04	Inorganic Chemistry Practical - II	3	6	40	10	50	2
	CHD3&4P. 05	Organic Chemistry Practical - II	3	6	40	10	50	2
	CHD3&4P. 06	Physical Chemistry Practical - II	3	6	40	10	50	2
	CHD4Pr	Project	4		32	8	40	4
	CHD4C13	Viva Voce (General)			35		35	4
		Total :	25		367	83	450	26

***The students may choose one elective from each of the following for semester II, semester III and semester IV.**

ELECTIVE PAPERS		
Sem & Paper	Paper Code	Title
II *Elective Paper I	CHD2E.01	Introduction To Computational Chemistry & Computational Drug Design
	CHD2E.02	Environmental Chemistry And Disaster Management
III *Elective Paper II	CHD3E.03	Introduction To Drug Chemistry
	CHD3E.04	Biochemistry And Biophysical Chemistry
IV *Elective Paper III	CHD4E.05	Drug Chemistry And Drug Design
	CHD4E.06	Medicinal Chemistry

Semesterwise Split-up of Marks

Sem	Hrs allotted	Marks for ESA	Marks for CA	Total Marks	Credit
I	25	240	60	300	16
II	25	360	90	450	22
III	25	240	60	300	16
IV	25	367	83	450	26
	100	**1207**	**293**	**1500**	**80**

2. **Project Work and Viva Voce**

a) Each student shall carry out a project work in one of the broad areas of theoretical/Organic/physical/environmental/inorganic chemistry for a period of minimum 12 weeks duration in the IVth semester under the supervision of a teacher of the department. A student may, in certain cases be permitted to do the project work in an industrial/research organization on the recommendation of the department coordinator. In such cases, one of the teachers from the department shall act as co-supervisor.

b) The candidate shall submit 2 copies of the dissertation based on the results of the project work at the end of the program.

c) Every student has to do the project work independently. No group projects are accepted. The project should be unique with respect to title, project content and project layout. No two project report of any students should be identical, in any case as this may lead to the cancellation of project report by the university.

d) The ESE of the project work shall be conducted by two external examiners. The evaluation of the project will be done at two stages.

i. Internal evaluation (supervising teacher/s will assess the project and award internal marks)

ii. External evaluation (by external examiners appointed by the university)

e) Pass conditions

i. The students shall declare to pass the project report course if she/he secures minimum of 40% marks (internal and external put together). In an instance of inability of obtaining a minimum of 40% marks, project work may be redone and the report may be resubmitted along with subsequent exams through parent department. There shall be no improvement chance for the marks obtained in the project report.

f) Assessment of different components of project may be taken as below

Internal (Viva) 20% of total		External (80% of Total)	
Components	**% of internal marks**	**Components**	**% of external marks**
Punctuality	10	Relevance of topic	5
Use of data	10	Statement of the topic	10
Scheme Organization of report	30	Methodology / reference / bibliography	15
Viva-voce	50	Presentation of facts/ figures / language style / diagrams etc	20
		Quality of analysis/ use of statistical tools	15
		Findings and recommendations	10
		Viva-voce	25

g) Viva voce shall be conducted by two examiners; both of them shall be external examiners. Viva-voce based on theory and practical papers of all semesters including elective papers.

3. Continuous assessment

a) This assessment shall be based on predetermined transparent system involving periodic written tests, assignments, seminars and attendance in respect of theory courses and based on tests, lab skill, record/viva and attendance in respect of practical courses.

b) The percentage of marks assigned to various components for internal is as follows

Theory		
No	**Components**	**% of internal marks**
1	Two test paper	40
2	Assignments	20
3	Seminars/Presentation of case study	20
4	Attendance	20

Practicals		
No	**Components**	**% of internal marks**
1	Two test paper	40
2	Lab skill	20
3	Records/viva	20
4	Attendance	20

4. Grading system

Seven point indirect grading system

The guidelines of grading is as follows

GRADING PATTERN

Sl. No	% of Marks	Grade	Interpretation	Range of Grade Points	Class
1	90 and above	O	Outstanding	9.0 - 10	First class with distinction
2	80 to below 90	A	Excellent	8.0 - 8.9	
3	70 to below 80	B	Very Good	7.0 - 7.9	First class
4	60 to below 70	C	Good	6.0 - 6.9	First class
5	50 to below 60	D	Satisfactory	5.0 - 5.9	Second Class
6	40 to below 50	E	Pass/Adequate	4.0 - 4.9	Pass
7	Below 40	F	Failed	0.0 - 3.9	Fail

5. Pass requirement

Those who secure not less than 40% marks (ESE and CA put together) for the all courses of a semester shall be declared to have successfully completed the semester. The marks obtained by the candidate for CA in the first appearance shall be retained (respective of pass or fail). The candidate who fails in theory unit shall reappear for theory unit only and the marks secured by them in practical unit, if passed in practicals will be retained. A candidate who fails to secure a minimum for a pass in a course will be permitted to write the same examination along with the next batch. For the successful completion of a semester a candidate should pass all courses and secure a minimum SGPA of 4. A candidate who secures minimum marks (40%) for a pass in a course will be permitted to write the same examination along with the next batch if he/she desires to improve his/her performance in ESE. There shall be no improvement chance for the marks obtained in the internal assessment. Improvement of a particular semester can be done only once the students shall avail the improvement chance in the succeeding year along with the subsequent batch. There shall be one improvement chance for a course.

6. Conduct of external examination

a) External examination in each semester shall be conducted after five months from the commencement of process. The board of examiners shall consist of two external examiners of the broad areas of theoretical / inorganic / organic / physical / environmental chemistry.

b) The board of examiners will value the theory papers, conduct practical and viva-voce examination and evaluate the project work. The answer script of each paper of external assessment shall be valued by two examiners and the average mark is awarded. If the marks awarded by the two examiners differ by more than 10% for a paper, a third examiner shall value the paper and the mark awarded by him shall be final. The project work shall be adjudicated by two external examiners. The practical examination, viva-voce and project evaluation will be conducted by two external examiners. The viva-voce examination will be based on the theory papers, practical papers, and project work as applicable.

c) The candidate shall be given one chance for improving the theory and practical papers of each semester by permitting him/her to appear for paper(s) along with the subsequent batch of students in accordance with the syllabus in course that time.

7. **Instructions to question paper setters**

The syllabus of each theory paper has four units. While setting the question papers, equal weightage is to be given to each of units for choosing the questions. Each question papers is of 3 hours duration and has four sections namely, section A, section B, section C and section D. Constituting a total of 60 marks for each of the papers. Question papers of practical examinations shall be prepared by the respective board of examinations.

Section	Criteria	Marks
A	8 questions (one word or one sentence), all must be answered	8 × 1 = 8
B	8 out of 12 questions (answer may be two or three sentences)	8 × 2 = 16
C	4 out of 8 questions (short paragraph questions)	4 × 3 = 12
D	4 out of 8 questions (essay type questions)	4 × 6 = 24
		Total = 60

Dr. Shibu P V
Chairman, Board of Studies in Chemistry (PG)
[Convener, Expert Committee]

SEMESTER-1

CHD1C.01 – THEORETICAL CHEMISTRY I

TOTAL HOURS: 72

UNIT -1

QUANTUM MECHANICS-I **18 HOURS**

Max Plank's Quantum Theory of Radiation - Photoelectric effect Black body radiation – Compton effect – Wave particle duality of matter-de-Broglie concept – Electron diffraction – Davison and Germer Experiment – Heisenberg's uncertainty Principle. Complex Numbers – definition - complex conjugate absolute values of a complex number – complex functions. Schrödinger wave mechanics – Deduction of Schrodinger equation from classical wave equation. Physical meaning of wave function. Normalized and orthogonal function. Elements of operator algebra: definition – linear and non – linear operators – commuting and non-commuting operators-vector operators – Laplacian operators and their expressions in spherical polar co- ordinates. Eigen functions and Eigen values – Hermitian operators. Formulation of quantum mechanics: The postulates of quantum mechanics – state function postulate – operator postulate – Eigen value postulate – Expectation value postulate – Postulate of time dependent Schrödinger equation stationary states and time independent Schrödinger equation.

UNIT – II

QUANTUM MECHANICS – II **18 HOURS**

Translational motion: Particle in a one-dimensional box-complete treatment – particle in a three dimensional box (rectangular and cubical box) – degeneracy. Quantum mechanics of vibrational motion One dimension Harmonic oscillator – complete treatment – Hermite polynomials – comparison of classical and quantum mechanical results. Quantum Mechanics of rotational motion: Particle on a ring – rigid rotator – the wave function in spherical polar co ordinates – complete treatment – Legendre polynomial – spherical harmonies – polar diagrams. Quantum mechanics of Hydrogen like atoms: potential energy of hydrogen like atoms – the wave equation in spherical polar co ordinates – solution of the R, θ, φ equations – Laguerre polynomials – associated Laguerre polynomials – Discussion of the wave functions – radical distribution function – orbitals and orbital diagrams – their significance.

UNIT – III

QUANTUM MECHANICS – III **18 HOURS**

Need of approximate methods in quantum chemistry: variation method – variation theorem with proof – variation treatment of the ground state of Hydrogen atom and Helium atom. Perturbation method: time independent first and second order correction to the energy and wave function – perturbation treatment of the ground state of Helium atom. Electron spin and atomic structure: spin functions and operators – spin orbit interactions – Angular momentum – commutation relations – operators Term symbols – Russel – Saunder's terms and coupling schemes – introduction to SCF methods – Hartree and Hartree – Fock's SCF.

UNIT – IV

CHEMICAL BONDING **18 HOURS**

Born – Oppenheimer approximation – essential principles of the M O method – M O treatment of Hydrogen molecule and the H_2^+ ion – valence bond treatment of ground state of hydrogen molecule – M O treatment of homonuclear diatomic molecules (quantitative) – Li_2, Be_2, N_2, O_2,O_2^+, O_2^-, F_2 and heteronuclear diatomic - LiH, CO, NO, HF – theory of chemical bonding for polyatomic molecules – Abinitio calculations – basic principles – HF calculations – basis sets – STO and GTO – Correlation diagrams – non crossing rules – Spectroscopic term symbols for diatomic molecules.

Localized bonds – hybridization and geometry of molecules – methane, water, ethene, acetylene (bond angle, dihedral angle, bond length and bond energy) – M O theory of conjugated systems and aromaticity (benzene)- bond order, charge density and free valence calculations – Brief discussion of bonding in metals.

REFERENCE

1. N Levine, *Quantum Chemistry 5th Ed*. Prentice Hall India
2. R. Anantharaman, *Fundamentals of Quantum Chemistry*, Mc Millan India
3. A. K. Chandra, *Introductory Quantum Chemistry* – 4th Ed. Tata Mc Graw Hill
4. D. A. McQurrie *Quantum Chemistry*, University Science Books
5. L. Pauling and W.B Wilson, *Introduction to Quantum Mechanics*, McGraw Hill
6. R. K. Prasad, *Quantum Chemistry4th Ed*. New Age International
7. P. W. Atkins, *Molecular Quantum Mechanics*, Oxford University Press
8. M.S.Day and J.Selbin, *Theoretical Inorganic Chemistry*, East West Books

– Tamas Veszpremi and Miklos Feber, *"Quantum Chemistry – Fundamentals to Applications"* Springer.

9. Quinn – "*Computational Quantum Chemistry – An Interactive Guide to Basis Set theory*"- Ane Books Pvt. Ltd.

SEMESTER – 1

CHD1C.02 – INORGANIC CHEMISTRY – 1

TOTAL HOURS: 72

UNIT – I **18 HOURS**

THEORETICAL BASIS OF ANALYSIS

Statistical treatment of errors – standard deviation for sample and population data – reliability of results, confidence level – comparison of results – the 't' and 'F' test – rejection of data Precipitation phenomena – precipitation trans homogenous solution – organic precipitants in inorganic analysis (a detailed study) – extraction of metal ions – nature of extractants – distribution law – partition coefficients – types of extraction and applications – chelometric titrations (a detailed study) – titration curves with EDTA – feasibility of EDTA titration – indicators for EDTA titration and its theory (a detailed study) – selective masking and demasking techniques – industrial application of masking

UNIT – II **18 HOURS**

ACIDS, BASES AND NON AQUEOUS SOLVENTS

A generalised acid base concept. Measure of acid base strengths – gas phase basicities – proton affinities – gas phase acidities – proton loss gas phase acidities – electron affinities – systematic of Lewis acid-base interaction – bond energies – steric effect – proton sponges. Solvation effects and acid base anomalies. Hard and soft acids and bases – classification – strength and hardness and softness – symbiosis – theoretical basis of hardness and softness – electron negativity and hardness and softness. Classification of solvents – properties of non aqueous solvents like NH_3 and H_2SO_4 – chemistry of molten salts as non aqueous solvent systems – solvent properties – room temperature molten salts – unreactivity molten salts - solution of metals – electrochemistry in non aqueous solution – hydrometallurgy

UNIT – III **18 HOURS**

NUCLEAR AND RADIATION CHEMISTRY

Nuclear models – shell, liquid drop, Fermi gas, Collective and optical models – equation of radioactive decay – half life and average life. Radioactive equilibrium – transient and secular equilibrium – types of nuclear reaction – spontaneous and reduced fission – neutron capture cross section and critical size – principles and working of GM, proportional , ionization and scintillation counters. Basic principles of nuclear reactors – types of reactors – PWR, VVER, BWR, PHWR, GCR, RBMK and LMFBR

Elements of radiation chemistry – introduction, interaction of ionizing radiation with matter. Bethe's equation for LET for charged particle due to collision with electron. Bremsstrahlung interaction of electromagnetic radiation with matter. Effects of ionizing radiation in water and aqueous solution. chemical dosimetry

UNIT – IV **18 HOURS**

BORON, PHOSPHORUS AND NITROGEN COMPOUNDS

The neutral boron hydrides – structure and bonding topological approach to boron hydride structure – styx number – synthesis and reactivity of neutral boron hydrides. Importance of icosohedral frame work of boron atoms in boron chemistry – closo, nido and arachno structure – Wades rule – mno rules – carboranes and metallocarboranes

Phosphorous sulphides – P_4S_3, P_4S_5, P_4S_7 and P_4S_{10} – preparation, properties, structure and uses. The phosphazenes (phosphonitrilic halides)

Sulphur nitrogen compounds – S_2N_2 and S_4N_4 – Polythiazl other S_XN_Y compounds. Their preparation properties, structure

REFERENCES

1) F A Cotton, Wilkinson, C A Murrillo and M Bochmann "Advanced Inorganic Chemistry 6th edition, John Wiley and Sons Inc
2) Bodie Douglas, Darl H Mc Daniel AND John J Alexander, Concepts and models of Inorganic Chemistry, John Wiley and Sons Inc 3rd edition
3) G N Jeffery, J Basette, J Mendham and R C Denny, Vogel's text book of quantitative chemical analysis (Vth edition), John Wiley and Sons
4) H Sisler, Chemistry of non aqueous solvents, Reinhold
5) J E Huhee, Inorganic Chemistry Principles of Structure and Reactivity, Person Education India
6) G Friedlander and J W Kennedy, Introduction to radiochemistry, John Wiley and Son Inc
7) S Glasston, Source book on atomic energy, Van Nonstrand
8) H J Arniker, Essentials of Nuclear Chemistry, New age international, New Delhi 4th edition 1995
9) J D Lee, Concise Inorganic Chemistry (IVth edition) Oxford University Press
10) S K Agarwal and Keemti Lal, Advanced Inorganic Chemistry, Pragati Prakashan 9th Edition 2009
11) B K Sharma, Instrumental Methods of Chemical Analysis, Goel publishing house, 2000
12) Duward F Shriver, Peter William, Atkins, Cooper Harold Langford, Inorganic Chemistry
13) M G Arora and M Singh, Nuclear chemistry
14) Walter D Loveland, David J Morrissey, Glenn T Seaborg, Modern Nuclear Chemistry
15) J E Huheey, Ellen A Keiter, Richard L Keiter, Inorganic Chemistry, Principles of Structure and Reactivity. 4TH Edition Addison-Wesley Publishing company

SEMESTER – I

CHD1C.03 - ORGANIC CHEMISTRY – I

TOTAL HOURS: 72

UNIT – I **18 HOURS**

AROMATICITY, STRUCTURE, REACTIVITY AND INTERMEDIATES

Aromaticity – principles of aromaticity, antiaromaticity, homo, hetero and non benzenoid aromatic systems – aromaticity of annulenes, mesoionic compounds, metallocenes, cyclic carbo cations and carbanions. Electronic effects – inductive, electromeric, mesomeric effects – hyperconjugation – Steric effect- influence of structural features on acidity, basicity and reactivity of organic compounds – structure, formation and properties of carbenes, nitrenes and arynes – singlet and triplet carbenes, nitrenes and arynes – singlet and triplet carbenes formations and reactions – Carbon free radicals: structure, formation and stability, radical reactions, auto oxidation and radical chain reactions – structure, stability, and formation of carbocations and carbanions

UNIT – II **18 HOURS**

STEREOCHEMISTRY AND MOLECULAR REARRANGEMENTS

Molecular chirality and steriochemical nomenclature – molecules with chiral axes and planes – molecular shape, topology and optical activity – Atropisomerism and its designation – racemization – resolution – prostereoisomerism – stereotopicity and enatiomeric excess – non carbon chiral centers – introduction to ORD, CD and their application in configuration and conformation – octant and axial and haloketones rules – conformational analysis of cyclo alkanes, decalins and their substituted derivatives.

Molecular rearrangements – mechanism, with evidence of Wagner-Meerwein, Pinacol, Demjanov, Hofmann, Curtius, Schmidt, Lossen, Beckmann, Wolff, Fries, Fischer-Hepp, Hoffmann-Martius, Von Richter, Orton, Bamberger, Smiles, Dienone-phenol, Benzilic acid, benzidine, Favorski, Stevens, Wittig, Sommlet-Hauser, Baeyer-villiger, and Borane rearrangements – Darkin reaction

UNIT – III **18 HOURS**

SUBSTITUTION AND ELIMINATION REACTIONS

Nucleophilic substitution at sp^3 carbon – its mechanism and stereochemical aspects – effects of solvent, leaving group and substrate structure – neighbouring group participation – nonclassical carbocations – aromatic nucleophilic substitution – benzyne, SN_1 and SNAr mechanisms

Elimination reaction leading to C=C bond formation and their mechanisms – stereo aspect of C=C bond formation – effect of leaving group and substrate structure – Hoffman and Saytzeff elimination, Solvolytic elimination reaction, thermal eliminations, other double bonds (C=N, C=O) by elimination. Triple bond elimination

UNIT – IV **18 HOURS**

PHOTOCHEMISTRY

Photochemical processes – energy transfer – sensitization and quenching – singlet and triplet and their reactivity, characteristics of photoreactions, typical photo reactions – photoreactions of carbonyl compounds, enes, dienes, and arenes – Norrish reaction of acyclic ketones, Patterno- Buchi, Burton, Photo-Fries and di-π methane rearrangement reaction – photo reactions of Vitamin D – Photochemistry of vision and photosynthesis – singlet oxygen generation and reactions – applications of photo reaction in laboratory and industrial synthesis

REFERENCE

1. D Nasipuri, Stereochemistry of organic compounds, Wiley Estern
2. P Y Bruice, Organic Chemistry, Prentice Hall
3. P Sykes, A guidebook to mechanism in organic chemistry, Pearson
4. S N Issacs, Physical organic chemistry, Longmann
5. M B Smith, March's Advanced Organic chemistry, 5th edtn, Wiley (or earlier editions of Jerry March)
6. F a Carey and R S Sundberg, Advanced organic chemistry, 4th Edtn, Part A and B, Kluwer
7. M A Fox and J K Whitesell, Organic chemistry, 2nd edtn, Jones and Barlett
8. C J Moody and W H Whitham, Reactive intermediates, Oxford University Press
9. I L Finar, Organic chemistry, Vol 2, Longmann
10. Maya Shankar Singh, Advanced organic chemistry: reactions and mechanism, Pearson

SEMESTER – I

CHD1C.04 - PHYSICAL CHEMISTRY- I

TOTAL HOURS: 72

UNIT-I **18 HOURS**

THERMODYNAMICS AND PHASE EQUILIBRIA

Third law of thermodynamics, Nernst heat theorem, determination of absolute entropies using third law, Residual entropy. entropy changes in chemical reactions. Thermodynamic equations of state. Maxwell relations and significance. Partial molar quantities - chemical potential- variation of chemical potential with T&P- determination of partial molar volume and enthalpy. Thermodynamic functions of ideal gases, real gases and gas mixtures- Entropy and free energy of mixing. Excess thermodynamic functions. Thermodynamics of irreversible processes with simple examples. Entropy production- rate of entropy production, entropy production in heat flow & diffusion- the phenomenological relations. The principle of microscopic reversibility, the Onsager reciprocal relations. Thermo osmosis and thermo molecular pressure difference, Thermoelectricity.

Phase equilibria: Physical equilibria involving phase transition-criteria for equilibrium between phase-Three component system- graphical representations-solid liquid equilibria- Ternary solution with common ion-Hydrate formation-compound formation-liquid-liquid equilibria-one pair of partially miscible liquids-two pairs of partially miscible liquids-three pairs of partially miscible liquids.

UNIT-II **18 HOURS**

ELECTROCHEMISTRY

Conductance measurements-Technique at high frequency and high voltage-Results of conductance measurements – ionic mobilities- Influence of pressure and temperature on ion conductance-Walden's equation- Abnormal ion conductance-Derivation of Debye-Huckel-Onsager equation- validity of Debye-Huckel-Onsager equation for aqueous and non-aqueous solution-Deviation from Onsager equation-Conductance ratio and Onsager equation-Dispersion of conductance at high frequencies-Debye-Falken effect-conductance with high potential gradients- Debye-Huckel limiting law and its various form, qualitative and quantitative tests of Debye-Huckel limiting equation. Osmotic coefficient- Ion- association-dissociation constant- Triple ion and conductance minima- Equilibria in electrolytes- Association constant-solubility product principle-solubility in presence of common ion- Activity coefficient and solubility measurement.

UNIT-III **18 HOURS**

ELECTRODICS

Different types of electrode-Electrochemical cell-concentration cell and activity coefficient. Determination of origin of electrode potential-liquid junction potential-the electrode double layer-electrode-electrolyte interface-Theory of multilayer capacity. Electric capillary- Lippmann

potential- Membrane potential- Polarization- electrolytic polarization. Dissolution and decomposition potential-concentration polarization. Butler–Volmer equation for simple electron transfer reaction-Transfer coefficient- Exchange current density Rate constants- Tafel equation and its significance- Principle of polarography. Polarization, overvoltage and polarography. Electrolytic polarization, dissolution and deposition potentials, concentration polarization. Decomposition voltage and its determination. Over voltage - hydrogen over voltage, oxygen overvoltage, metal deposition over voltage and their determination. Theories of over voltage - Ionic diffusion as the slow process - dropping mercury electrode, the half wave potential. Electrode kinetics.

UNIT-IV **18 HOURS**

CORROSION

Definition and importance of corrosion. Corrosion science and engineering. Economic aspects of corrosion- global and Indian situations. Causes of corrosion- Change in Gibbs free energy. Pitting-Bedworth ratio. Electrochemical mechanism-The dry cell analogy and Faraday's law-Definition of cathode and anode-Types of cell- Types of corrosion damage. Thermodynamics of corrosion and electrode potentials. EMF of a cell-measurement of emf - calculation of half cell potential-Nernst equation. Basis of Pourbaix diagrams- Diagrams of water, Fe and Al. Limitations of Pourbaix diagrams.

Kinetics of corrosion- Polarization and corrosion rate. Measurement of corrosion rate. Measurement of polarization- causes of polarization. Calculation of IR drops in a electrolyte. Influence of polarization on corrosion rate. Polarization diagram of corroding metals. Calculation of corrosion rate from polarization data. Electrochemical Impedance Spectroscopy. Theory of cathode protection. Passivity.

REFERENCES

1. Rastogi and Misra-"An Introduction to chemical thermodynamics-6thedition"– Vikas publishing.
2. S. Glasstone-"Thermodynamics for chemists"–Affiliated East West publication.
3. Lewis and Randal-"Thermodynamics"-McGrawHil.
4. Daniels and Alberty-"Physical Chemistry"- John Wiley.
5. "Mathematics of Physics and Chemistry"-VolMargeman and Murphy.
6. S. Glasstone-"Theoretical electrochemistry"-East West Books
7. L.I. Anthropov-"Theoretical electrochemistry"-Mir publishers.
8. Bockris and Reddy-"Modern electrochemistry"-Springer
9. G.W. Castelon "Physical chemistry"-Narosa
10. I. Pregogine-"Introduction of Irreversible to thermodynamics process"-Interscience
11. G.M.Barow- Physical Chemistry- TataMcGrawHil.

12. Duta K.Robin "Physical Chemistry "Ane Books
13. Winston Revie and Herbert Uhlig Corrosion and corrosion control:(Wiley) Edited by Sheir, Jarman and Burstein Corrosion Control Volume 2
14. Fontana and Greene Corrosion engineering

SEMESTER II

ELECTIVE PAPER I

CHD2E.01- INTRODUCTION TO COMPUTATIONAL CHEMISTRY & COMPUTATIONAL DRUG DESIGN

Total Hours: 72

Unit 1: Introduction to Computational Chemistry — 10 Hours

Theory, computation & modeling – Definition of terms. Need of approximate methods in quantum mechanics. Computable Quantities – structure, potential energy surfaces and chemical properties. Cost & Efficiency – relative CPU time, software & hardware. Classification of computational methods.

UNIT 2: *ab intio* Methods in Computational Chemistry — 10 Hours

Review of Hartree – Fock method for atoms, SCF treatment of polyatomic molecules; Closed shell systems - restricted HF calculations; Open shell systems – ROHF and UHF calculations; The Roothan – Hall equations, Koopmans theorem, HF limit & electron correlation, Introduction to electron correlation (post -HF) methods: Møller Plesset Perturbation Theory, Configuration Interaction, Coupled Cluster and semi empirical methods (elementary idea only).

UNIT 3: Density Functional Methods — 10 Hours

Introduction to density matrices, N-representability & V-representability problems, Hohenberg – Kohn theorems, Kohn-Sham orbitals, Exchange correlation functionals– Thomas-Fermi- Dirac model, Local density approximation, generalised gradient approximation, hybrid functional. Comparison between DFT and HF methods.

UNIT 4: Basis Set Approximation — 10 Hours

Hydrogen-like, Slater-type & Gaussian type basis functions, classification of basis sets – minimal, double zeta, triple zeta, split-valence, polarization & diffuse basis sets, contracted basis sets, Pople-style basis sets and their nomenclature, correlation consistent basis sets, basis set truncation error, effect of choice of method / basis set (model chemistries) on cpu time.

UNIT 5: Quantum Chemical Calculations — 20 Hours

Preparation of 2D molecules using ChemSketch and Chemdraw - Molecular editor and visualization in 3D using Avogadro / GaussView / McMolPlt / ChemCraft. Simple calculations using Gaussian / GAMESS / Turbomole / Orca quantum chemistry programme – The structure of an input file, Types of keywords, Specification of molecular geometry using (a) Cartesian coordinates and (b) Internal coordinates. The Z-matrix, Z- matrices of some simple molecules like H_2, H_2O, formaldehyde, ammonia and methanol etc. Calculation of single point energy – minimization of molecular structures by geometry optimization - characterizing stationary points – interpreting normal mode information – calculation of IR and Raman spectra - modeling thermochemistry .

UNIT 6: Computational approaches to drug design and discovery — 12 Hours

General approach to discovery of new drugs - Drug Discovery Cycle, The Lead compound, Pharmacophore, database resources for drug discovery - chemical databases, physiochemical principles of drug action - ADME and Toxicity, Virtual Screening, Molecular Docking, Structure

and Ligand Based Drug Designing. Structure comparison and overlays – identification of active conformations - Tools for Molecular Visualization and Analysis: RASMOL, PYMOL - Molecular Electrostatic Potentials - Molecular Modeling and Docking: Automated screening of databases for lead compounds - *De novo* drug design

References:

1. C. J. Cramer, *Essentials of Computational Chemistry: Theories and models,* John Wiley & Sons 2002.
2. Frank Jensen, *Introduction to Computational Chemistry,* John Wiley & Sons LTD1999.
3. J. Foresman & Aelieen Frisch, *Exploring Chemistry with Electronic Structure Methods*, Gaussian Inc., 2000.
4. David Young, *Computational Chemistry- A Practical Guide for Applying Techniques to Real-World Problems"*, Wiley -Interscience, 2001.
5. Errol G. Lewars, *Computational Chemistry: Introduction to the theory and applications of molecular quantum mechanics,* 2 nd edn, Springer2011.
6. I.N. Levine, *Quantum Chemistry*, 6th Edition, Pearson Education Inc., 2009.
7. P.W. Atkins & R.S. Friedman, *Molecular quantum mechanics*, 4th Edition, Oxford University Press, 2005.
8. W. Koch, M.C. Holthausen, *"A Chemist's Guide to Density Functional Theory"*, Wiley-VCH Verlag 2000.
9. D. Baxivanis and Foulette - Bioinformatics: A Practical Guide to the Analysis of Genes and Proteins, Wiely Indian Edition, 2001.
10. T K Attwood, D J parry-Smith, Introduction to Bioinformatics, Pearson Education, First Edition, 11th Reprint 2005

SEMESTER II

ELECTIVE PAPER I

CHD2E.02 - ENVIRONMENTAL CHEMISTRY AND DISASTER MANAGEMENT

TOTAL HOURS: 72

UNIT–I **18HOURS**

ENVIRONMENTAL AND ATMOSPHERIC POLLUTION

Components of environment, Factors effecting environment – segments of environmental. Atmosphere – composition and structure. Soil – composition and process of soil formation. Hydrosphere – sea water and river water composition. Environmental pollution – pollutant definition – origin, classification and types of pollution. Air pollution – sources (industrial, automobiles) – effect of SO_2, NO_X, CO, H_2S, smoke, hydrocarbons on human and plant systems. Cause and consequence of acid rain, green house effect, ozone depletion and photochemical smog. Air pollution control method. Air pollution accident – Bhopal tragedy

UNIT–II **18 HOURS**

a) Soil, water, thermal and radioactive pollution

Soil pollution sources – effect of fertilizers as soil utilization and agricultural work, pesticide and herbicides. Control methods. Water pollution – sources, effect of pollutants – oxygen deficiency, eutrophication. Water quality criteria for industrial and domestic use. Sewage treatment – industrial waste water treatment, experimental determination DO, COD, and BOD. ISI standard of drinking water

Thermal and radioactive pollution. Sources and control of thermal pollution. Sources and effects of radioactive pollution

b) Instrumental methods in chemical analysis

A brief study i) AAS, ii) X-ray fluorescence, iii) gas chromatography and iv) ion selective electrodes

UNIT–III **18 HOURS**

INTRODUCTION TO DISASTERS

Concepts, and definitions (Disaster, Hazard, Vulnerability, Resilience, Risks). Disasters: Classification (Natural and Manmade), Causes, Impacts (including social, economic, political, environmental, health, psychosocial, etc.). Differential impacts – in terms of caste, class, gender, age, location, disability. Global trends in disasters, urban disasters, pandemics, complex emergencies, Climate change

UNIT–IV **18 HOURS**

DISASTER MANAGEMENT

Disaster management mechanism: Concepts of risk management and crisis management, Disaster management cycle, Response and Recovery, Development, Prevention, Mitigation and Preparedness, Planning for disaster management: Strategies for disaster management planning, Steps for formulating a disaster risk reduction plan, Disaster management Act and Policy in India, Organizational structure for disaster management in India, Preparation of state and district disaster management plans, Technologies for Disaster Management: Remote Sensing, GIS and GPS

REFERENCES

1. B K Sharma and H Kaur, Thermal and radioactive pollution, Krishna Prakashan Mandir, Meerut
2. B K Sharma and H Kaur, Water pollution, Krishna Prakashan Mandir, Meerut
3. T H Y Tebbut, Principles of water quality control A,Butterworth-Heinemann
4. Anil K De, Environmental chemistry 4thedtn. New age International PvtLtd
5. Cleaning our environment-A chemical perspective 2ndedtn, American Chemical Society
6. S K Banerjee, Environmental chemistry, Goel Publishing house, Meerut
7. L W Moore and E A Moore, Environmental chemistry, McGraw Hill Publication, New York
8. Gary W Vanloon and Stephen J Duffy, Environmental chemistry-A global perspective, Oxford University Press
9. Baily Clark, Ferris Kraus and Strong, Chemistry of the environment, Elsevier
10. Alexander, D. *Natural Disasters,* ULC press Ltd, London,1993.

SEMESTER – II

CHD2C.05 – THEORETICAL CHEMISTRY II

TOTAL HOURS: 72

UNIT – I **18 HOURS**

MOLECULAR SYMMETRY, GROUPS, MATRICES

Symmetry elements and symmetry operations in molecules – mathematical groups, point groups and their symbols – sub group – relation between orders of a fine group and its sub group – isomorphism. Abelian and cyclic groups - group multiplication tables – classes in a group and similarity transformation – Matrices – addition and multiplication of matrices – inverse of a matrix character of a matrix block diagonalisation – matrix form of symmetry operations – Matrix representation of symmetry operations – representation of groups – construction of representation using vectors and atomic orbital as basis – Representation generated by Cartesian coordinates positioned on the atoms of a molecule ($H_2O$and SO_2 as examples) – reducible and irreducible representations – construction of irreducible representation by reduction.

UNIT II **18 HOURS**

THEORY OF MOLECULAR SYMMETRY AND APPLICATIONS OF GROUP THEORY

Great Orthogonality Theorem (GOT) (without proof) – properties of irreducible representations - construction of irreducible representation using GOT – construction of character tables (C_2v, C_2h, C_3v, C_4v). Applications to molecular vibrations – symmetry aspects of molecular vibrations – vibrations of polyatomic molecules – selection rules for vibrational absorption – complementary character of 1 R and Raman spectra – determination of the number of active 1 R and Raman Lines. Applications to chemical bonding – construction of hybrid orbitals – BF_3 CH_4, PCI_5 as examples- transformation properties of atomic orbital. Application to MO theory of H_2O, NH_3 and octahedral complexes.

UNIT – III **18 HOURS**

SPECTROSCOPY

General theory: electromagnetic radiation, regions of the spectrum, interaction of electromagnetic radiation with matter and its effect on the energy of molecules – Natural line width and broadening. intensity of spectral lines – Rotational, vibrational and electronic energy levels and selection rules – transition moment integral Microwave spectroscopy: Classification of molecules – rotational spectra of diatomic and polyatomic molecules – Rigid and non-rigid rotator models – Determination of bond lengths – isotope effect on rotation spectra – applications.

Vibrational and vibration – rotation spectra : Vibrational energies of diatomic molecules – interaction of radiation with vibrating molecules – anharmonicity of molecular vibrations, fundamental, overtones and hot bands – Degree of freedom of poly atomic molecules and nature of molecular, vibrations (eg. CO_2 and H_2O). vibration – rotation spectra of diatomic and

polyatomic molecules selection rules – determination of force constant.
Raman Spectroscopy : Theory of Raman spectra (classical and quantum mechanical theory) – pure rotational vibrational Raman spectra, vibrational –rotational Raman spectra, selection rules – mutual exclusion principle – Applications of Raman and I R spectroscopy in elucidation of molecular structure (eg. H_2O, N_2O and CO_2 molecules)

UNIT –IV **18 HOURS**

SPECTROSCOPY II

Electronic spectra : Electronic spectra of diatomic molecules – vibrational coarse structure and rotational fine structure of electronic spectrum – Franck – Condon principle – Types of electronic transitions – Fortrat diagram – Dissociation and pre – dissociation – calculation of heat of dissociation.

Nuclear Magnetic Resonance Spectroscopy: General theory – magnetic properties of nuclei – theory and measurement techniques – population of energy levels – solvents used –chemical shift and its measurement – factors affecting chemical shift – Nuclear resonance – Relaxation methods – integration of NMR signals – spin sin coupling – coupling constant j and factors affecting it – shielding and de shielding – chemical shift assignment of major functional groups – classification (ABX, AMX, ABC, A_2B_2 etc) spin decoupling – Application to the study of simple molecules. NMR studies of nuclei other than Proton: ^{13}C chemical shift and factors affecting it- ^{19}F and ^{31}P NMR.

REFERENCE

1. F A Cotton, *"Chemical Applications of Group Theory"* Wiley Eastern.
2. L H Hall "*Group Theory and Symmetry in Chemistry",* McGraw Hill.
3. V Ramakrishnn and M S Gopinathan, *"Group Theory in Chemistry"* Vishal Publications, 1992.
4. Banwell and Mc Cash "*Fundamentals of Molecular Spectroscopy",* Tata McGraw Hill
5. G Aruldas *"Molecular Structure and Spectroscopy",* Prentice Hall,
6. Manas Chanda *"Atomic Structure and Chemicals Bonding including Molecular Spectroscopy, 4th Edn,"* Tata McGraw Hill
7. Barrow "*Molecular Spectroscopy,"* McGraw Hill.
8. P W Atkins *"Physical Chemistry*," ELBS
9. S Swarnalakshmi, T Saroja and R M Ezhilarasi *"A Simple Approach to Group Theory in Chemistry"* – Universities Press
10. Thomas Engel "*Quantum Chemistry and Spectroscopy"* – Pearson.
11. Quinn "*Computational Quantum Chemistry – II : The Group Theory Calculator"* – Ane Books
12. H.Kaur "Spectroscopy" 3rd Edition Pragati Prakasan Meerut

SEMESTER – II

CHD2C.06 - ORGANIC CHEMISTRY – II

TOTAL HOURS: 72

UNIT – I **18 HOURS**

PERICYLIC REACTIONS

Symmetry properties of MOs – LCAO-MO theory of simple conjugated polyenes and cyclic polyenes – classification of pericyclic reactions – Woodward Hoffmann's rule, mechanism and stereo course of electrocyclic, cyclo addition and sigmatropic reactions. Analysis of electrocyclic and cyclo addition reactions by FO and Correlation diagram methods. Analysis of sigma tropic reaction by FO method. [3,3] migrations – Claisen and Cope rearrangements, stereo aspects of Diels Alder reaction – Retro Diels Alder reactions – fluxional molecules, ene, chelotropic and cis elimination reactions – synthetic applications.

UNIT – II **18 HOURS**

C–C AND C=C BOND FORMATION REACTIONS

Name reactions – Mannich, Simon-Smith, Stork enamine, Wittig-Horner, Peterson, Heck, McMurray, Vilsmeier and Haack reactions. Michael reactions, Prevost and Woodward hydroxylation of alkenes, Barton and Shapiro reaction, Sharpless asymmetric epoxidation, ring formation by Dieckmann, Thorpe and Acyloin condensation. Robinson ring annulations, reduction and oxidation in synthesis – catalytic hydrogenation. Alkali metal reduction. Birch reduction. Wolff-Kishner reduction, Huang-Milon modification. Clemmenson reduction. Boranes, LAH, DIBAL, sodium borohydride as reductants. Oppenauer oxidation. HIO_4, OsO_4 and mCPBA and their applications.
Synthetic applications of following reagents – Gillman reagent, LDA, 1, 3 dithiane, DDQ, DDC, sEo2, Bakers yeast, NBS, Wilkinsons's catalyst

UNIT – III **18 HOURS**

CHEMISTRY OF BIOMOLECULES AND NATURAL PRODUCTS

Steroids – classification of steroids, structure and biological importance of cholesterol, ergosterol, ergocalciferol – nomenclature, reactivity and stereochemistry of steroidal systems – stereochemistry and structure elucidation of cholesterol. Structure, synthesis and biological activity of testosterone and androsterone, estrone, progesterone. Structure and biological importance of cortisone and corticosterone. Bio synthesis of cholesterol. Structure of pencillins – synthesis of paracetamol, Phenobarbital, diazepam, sulphamethoxazole, and cholaramphenicol.

Structure and synthesis of beta-carotene, anthocyanin, flavones, isoflavone, cyanin and quercetin. Biosynthesis of terpenes (alpha-pinene and camphor) and alkaloids (ephedrine, dopamine, conine and nicotine)

Terpenoids – structure of Ocimene, Allo-Ocimene, menthol, caryophyllene (with brief introduction). Structure and synthesis of Alfa Pinene and Camphor

Alkaloids classifications – Hoffmann, Emde and Von Braun degradation in alkaloid chemistry,

structure elucidation of Papavarine and Morphine. Synthesis of Papaverine and Quinine.

UNIT – IV **18 HOURS**

CHEMISTRY OF POLYMERS AND BIOPOLYMERS

Plastic technology; molding, extrusion and other processing methods – additives and compounding – fiber technology: textiles and fabrics properties – fiber after treatment – mercerization – regenerated cellulose – viscose rayon – cellophane – cellulose acetate – elastomer technology: natural and synthetic rubbers – vulcanization – reinforcement – elastomer properties and compounding – structure of natural rubber.

Preparation, properties, structure and application of the following: [polyethylene, polypropylene, polystyrene, polychloroprene, PVC, Teflon, phenol formaldehyde, urea formaldehyde resins, polyurethanes, amino resins, nylons, polyester and caprolactam based polymers

Biological activities of vitamins, A, B, C and biotin, structure and synthesis of vitamin A and C, structure only of vitamin B complex (B_1, B_2 and B_6 and Biotin)

FMOC, BOC, Z, Trityl phthalimide and benzyl protecting groups – peptide bond formation by carbodiimide and active ester methods in SPPS. Chemistry of nucleic acid bases A, G, C, T and U and their synthesis, structure of adenosine and cytidine, structure of starch, cellulose, glycogen and chitin with brief introduction.

REFERENCES

1. F A Carey and R J Sundberg, Advanced organic chemistry part B, Plenum Press (2007)
2. M B Smith, Organic synthesis 2nd edtn, McGraw Hill, Inc (2001)
3. S Warren, Designing of organic synthesis
4. J Fuhrhop and G Penzlin, Oragnic synthesis 2nd edtn
5. Carruthers, Some modern methods of organic synthesis
6. H O House, Modern synthetic reactions
7. Fieser and Fieser, Reagent in organic synthesis
8. R O C Norman, Principles of organic synthesis
9. J March, March's advanced organic chemistry
10. J Clayden, Greeves, Warren and Wothers, Organic Chemistry, Oxford University Press
11. Ahluwalia Mukhergi and Singh, Organic reaction mechanisms
12. Maya Shankar Singh, Advanced organic chemistry: reactions and mechanisms,

Pearson

13. Peter Sykes, A guide book to mechanism in organic chemistry, 6th edn, Pearson
14. I M Cambell, Introduction to synthetic polymers, Oxford Scientific Publications
15. G S Misra, Introduction to polymer chemistry, New AGE
16. Naren, Polymer as aids in organic chemistry, Academic Press London
17. I L Finar, Organic Chemistry Volume 2, Pearson Education.

SEMESTER-II

CHD2C.07 - PHYSICAL CHEMISTRY- II

TOTAL HOURS: 72

UNIT-I **18HOURS**

STATISTICAL THERMODYNAMICS

Basic principles: permutation- probability concept Thermodynamic probability- Stirlings approximation, Macrostates and microstates-Derivation of Boltzmann distribution law – Partition function- physical significance-, phase space, Ensembles- partition function- Distinguishable and Indistinguishable molecules- Partition function and thermodynamic function-Separation of partition function - Translational, Rotational, vibrational and electronic partition function. Thermal de-Broglie wavelength. The calculations of thermodynamic functions and equilibrium constants - Equation of state – Sackur Tetrode equation-Statistical formulation of third law of thermodynamics. Heat capacity of gases-classical and quantum theories - Heat capacity of Hydrogen – ortho and para Hydrogen.

UNIT-II **18 HOURS**

LIQUID STATE AND QUANTUM STATISTICS

The atomic crystals: Einstein's theory of atomic crystal - Debye's modification of Einstein's model. Need for Quantum statistics-Bose-Einstein statistics - Bose-Einstein condensation - Liquid Helium- super cooled liquids Fermi- Dirac distribution- Examples of particles-Application of free electron gas. Thermionic emission. Comparison of three statistics. X-ray diffraction study of simple liquids and their structure- Configurational partition function for liquids- Theories of liquid state: free volume and Van der Waals theories- -communal entropy-specific heat of liquids. Liquid crystals - Mesomorphic state-types, examples and application-Theories of liquid crystals-photoconductivity of liquid crystals.

UNIT-II **18 HOURS**

SOLID STATE

Perfect and imperfect crystals, intrinsic and extrinsic defects-point defects, line and plane defects, vacancies-Schottky defects and Frenkel defects- colour centres, non-stoichiometric defects. Imperfection and physical properties of solids- Electrical properties- electrical conductivity- Hall effect- dielectric properties piezoelectricity- Ferro electricity and conductivity- Magnetic properties- diamagnetism- paramagnetism- Ferro, antiferro and ferrimagnetisms- Electronic structure of solids-band theory, Refinement to simple band theory - k-space and Brillouin Zones, superconductivity in metals- BCS theory- Meissner effect -type I & II superconductors- Transition metal Oxides (Spinels, Perovskite).

UNIT-IV **18 HOURS**

CRYSTALLOGRAPHY

Characterisation of solids, types of solids- isomorphism and polymorphism- laws of crystallography- lattice types-crystal and diffraction of X-rays-Laue equation- Bragg's Law-Mi**ll**er indices- Bragg Method-Debye-Scherrer method of X-ray structure analysis of crystals, indexing of reflections, identification of unit ce**ll**s from systematic absence in diffraction pattern-structure of simple lattice - X-Ray intensities-structure factor and its relation to intensity and electron density-phase problem.

REFERENCES

1. M.C. Gupta-"Elements of statistical Thermodynamics-New age international.
2. L.K Nash-"Elements of statistical Thermodynamics-Addision Wesley publishing Co.
3. Kistinand Sorfuran-"A course on statistical thermodynamic"-Academic 1971.
4. D.A. McQuarrie-"Statistical thermodynamic"-HarperandRow1973.
5. D.K. Chakrabarty-"Solid state chemistry"-New age publication.
18. I.V. Azaroof-"Introduction to solids"-Mc Graw Hill.
19. Lesley E. Smart and Elaine A. Moore. "Solid state chemistry an introduction" Third edition, 2005. Taylor and Francis group.
20. A.R. West, Solid State Chemistry and its Applications, (1984) John Wiley and Sons, Singapore
21. Uri Shmueli. "Theories and techniques of crystal structure determination" Oxford University press, 10.2007.
22. Christopher Hammond. "The basics of crysta**ll**ography and diffraction" Third edition, 2009, Oxford University press.
23. Molewyn Hughes-"Physical chemistry"-Pergamon press.
24. S.Glasstone and H.S.Taylor-"Treatise of Physical Chemistry"-Dvan Nostrand.

CHD1&2P.01 INORGANIC CHEMISTRY PRACTICAL– I

(1st and 2nd semester)

TIME: 108 HOURS

Credit 2

1) Separation and identification of four metal ions of which two are rare/ less familiar such as Tl, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li (interfering acid radicals not present). Confirmation by spot test. (Minimum 10 mixtures are to be recorded)
2) Volumetric estimation
    a) EDTA – Al, Ca, Cu, Ni, Co, Hardness of water
    b) Cerimetry – Fe(II), nitrate
    c) Potassium iodate-iodide, Sn(II)
3) Colorimetric determination of Cr, Fe, Ni and Mn

REFERENCE

1) G H Jeffrey, J Bassette, J Mendham and R C Denny, Vogel's text book of quantitative inorganic analysis, Longman, 1999
2) G S Vehla, Vogel's quantitative inorganic analysis (7th edition), Longman 2001

CHD1&2P.02 ORGANIC CHEMISTRY PRACTICAL – I

(I^{st} and 2^{nd} semester)

TIME: 108 HOURS

Credit 2

1) General methods of separation and purification of organic compounds with special reference to
    a) Solvent extraction (One example must be recorded)
    b) Fractional crystallization (One example must be recorded)
    c) Sublimation (One example must be recorded)
2) Analysis of organic binary mixtures: Separation and identification of organic binary mixtures containing one component with at least two substituents (a study is expected to analyze at least 8 different binary mixtures). Identification of the compounds by the determining the physical constants of the components of the mixture and melting point of the derivatives (by referring tables)
3) Preparation of organic compounds: Single stage preparation by reaction involving nitration, halogenations, oxidation, reduction, alkylation, acylation, condensation and rearrangement (a student is expected to prepare at least 10 different organic compounds by main use of the reaction given above)
4) Preparation, assay including limit tests prescribed in the IP/BP of the following drugs: sodium salicylate, calcium lactate, yellow mercuric oxide, ferrous fumarate, ferric ammonium citrate, potassium antimony citrate, boric acid, light magnesium carbonate, and sodium citrate. Expectorants and emetics (NH_4Cl, antimony potassium tartrate), Respiratory Stimulants $(NH_4)_2CO_3$, Dental products (Dicalcium Phosphate, Sodium Fluoride) Gastrointestinal agents: $MgSO_4$ (Any two)
5) Assay, test for identity and purity of the following synthetic drugs:
    Aspirin, Paracetamol, Ibuprofen, hexamine, Boric acid, Ferrous Fumarate, Isoniazid, Calcium lactate, Calcium gluconate (Any two).

References

1. A I Vogel, A text book of practical organic chemistry, Longman
2. A I Vogel, Elementary practical organic chemistry, Longman
3. F G Mann and B C Saunders, practical organic chemistry, Longman
4. Shriner and Others, Systematic identification of organic compounds
5. Dey, Sitharaman and Govindachari, A laboratory manual of organic chemistry
6. P R Singh, D C Gupta and K S Bajpal, Experimental organic chemistry vol I and II
7. Vishnoi, Practical organic chemistry
8. Fieser, Experiments in Organic chemistry
9. Experimental Pharmaceutical Organic Chemistry, A Benchtop Manual by K. S. Jain, P. B. Miniyar & T. S. Chitre, 2nd Edition Carrier publications,.
10. Organic Chemistry, G. Marc Loudon, 4th Ed., Oxford University Press, 2004.
11. British Pharmacopoeia Commission, British Pharmacopoeia:2012 Edition, Bernan Assoc, 2011
12. A.O. Bentley, J.E. Driver, Bentley and Driver's Textbook of Pharmaceutical Chemistry, 7th Edn., Oxford University Press, 1960.

13. G.L. Genkins, A.M. Knevel, F.E. Di Gangi, Quantitative Pharmaceutical Chemistry, 7th Edn., McGraw Hill, 1977.
14. K.A. Connors, A Textbook of Pharmaceutical Analysis, John Wiley & Sons, 2007.
15. Indian Ministry of Health and Family Welfare, Indian Pharmacopoeia 1996, Controller of Publication, 2000.

CHD1&2P.03 PHYSICAL CHEMISTRY PRACTICAL – I

(I^{st} and 2^{nd} semester)

TIME: 108 HOURS

Credit 2

(A minimum of 20 experiments to be done covering all units)

1. Phase rule
   a) Distribution law: partition of iodine between water and carbon tetrachloride. Equilibrium constant of $I^- + I_2 \rightarrow I_3^-$. Concentration of unknown KI. Partition of ammonia between water and chloroform. Equilibrium constant of $Cu^{2+} + 4NH_3 \rightarrow [Cu(NH_3)_4]^{2+}$. Partition of aniline with benzene and water. Hydrolysis constant of aniline hydrochloride. Association of benzoic acid in benzene
   b) Solid and liquid equilibria: construction of phase diagram of simple eutectics, systems with congruent melting points and solid solutions. Determination of composition of unknown mixtures. Analytical and synthetic methods for the determination of solubilities and heat of solution
   c) Partially miscible liquids: critical solution temperature, influence of impurities on the miscibility temperature (KCl, NaCl and /or succinic acid). Determination of composition of unknown mixtures.
   d) Completely miscible systems: construction of phase diagram of two component liquid system. Zeotropic and azeotropic
   e) Three component systems: with one pair of partially miscible liquids. Construction of phase diagrams of tie lines. Compositions of homogenous mixtures.
2. Solubility and Heat of solution Heat of solution from solubility data – analytical method and graphical method (ammonium oxalate and succinic acid)
3. Molecular weight determination Molecular weight determination: Cryoscopic method and transition temperature method. Molecular weight of a solid using a solid solvent by cooling curve method (solvents – naphthalene, biphenyl, diphenylamine, p-dichloro benzene). Molecular weight determination by study of depression in transition temperature (sodium acetate, sodium thiosulphate and strontium chloride)
4. Cryoscopic study: Study of $2KI + HgI_2 \rightarrow K_2HgI_4$ Reaction in water and determination of concentration of KI solution
5. Refractometry: Determination of molar refraction of pure liquids (water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol). Determination of composition of mixture (alcohol-water, glycerol-water, KCl-water)
6. Viscosity: Determination of viscosity of pure liquids (water, methanol, ethanol, glycerol, benzene, nitrobenzene, carbon tetrachloride). Composition of binary liquid mixture benzene - nitrophenol, water-alcohol). Determination of molecular weight of a polymer (polystyrene in toluene)
7. Potentiometry: Electrode potential of Zn and Ag electrodes in 0.1 M and 0.001 M solutions at 25 °C and determination of standard potentials. Mean activity coefficient of an electrolyte at different molalities by EMF method. Dissociation of strength of the given HCl solution by the different potentiometric titration. Dissociation constant of acetic acid in DMSO, DMF, acetone and dioxin by titrating with sodium hydroxide. Potentiometric titration. Acid base titration, redox titration, mixture of HCl and CH_3COOH.

8. Determination of pKa valued of drug molecules.
9. Determination of pKa values at different pH conditions.

Reference

1. A Findlay and J A Kitchener, Practical physical chemistry, Longman
2. F Daniels and J H Mathews, Experimental physical chemistry, Longman
3. A M James, Practical physical chemistry, J A Churchil
4. H H Williard, L L Merritt and J A Dean, Instrumental methods of analysis, Affiliated East West press
5. D P Shoemaker and C W Garland, Experimental physical chemistry, McGraw Hill
6. W G Palmer, Experimental physical chemistry, Cambridge University Press

SEMESTER III

ELECTIVE PAPER II

TOTAL HOURS: 72

CHD3E.03 - INTRODUCTION TO DRUG CHEMISTRY

Unit 1: Pharmacology 18 Hours

Drugs and Drug targets- Enzymes: active sites, mechanism of catalysis, Enzyme inhibitors, Enzyme selectivity, Receptors ligand gated ionic channels, G-Protein coupled receptors, Kinase linked receptors. Carrier Proteins, Structural Proteins, Nucleic acids, Lipids and carbohydrates and DNA as drug targets.

Structure activity relationship, Binding interactions, Functional groups as binding groups, Concept and definition of pharmacophore

Pharmacokinetic principles: absorption, distribution, metabolism and excretion of drugs. Dose of drugs and routes of administration. .Drug dosing, drug half life, Steady state concentration, Drug tolerance, Bioavailability, Drug delivery.

Pharmacodynamic principles : Examples of agonists, allosteric modulators, Antagonists, Partial agonists, Inverse agonists, Desensitization and sensitization, Tolerance and dependence, Affinity, efficacy and potency.

Dose response relationships, unusual and adverse responses of drugs, structurally specific and nonspecific drugs. Ferguson's principle.

UNIT 2: Toxicology and Biotransformations 12 Hours

General concepts of toxicity, Acute, subacute & chronic toxicity tests, teratogenicity & carcinogenicity, LD50, ED50, MIC- anti infectives, habituation & addiction

Biotransformation of Drugs, factors affecting biotransformation, site of biotransformation, Effect of biotransformation on the biological activity of drugs, alterations in Phase I biotransformations Biotransformation- Oxidation, reduction, hydroxylation, hydrolysis-illustrate reactions and mechanism with specific drugs molecules. Phase II biotransformations - Glucuronidation, sulfation, conjugation with glutathione, acetylation methylation- illustrate with suitable drug molecules.

UNIT: 3 Anti-infective Agents: 14 Hour

Sulphonamides- structure, chemistry, SAR and mechanism of action Sulfadiazine, sulfamethoxole, sulfones.

Antifungal agents: study of the following- Amphotericin B, ketoconazole, clotrimazole.

Other Antiprotozoal agents: Chemistry, mechanism of action and therapeutic uses of Anti Amoebic and Antihelmintics

Antiviral agents: Antiviral drugs- mode of action and therapeutic uses, Chemistry and mechanism of action of- amatidine, ribavirin.

Synthesis of - Sulphanilamide

UNIT 4: Chemotherapeutic Agents **14 Hours**

Antibiotics- Classification, mechanism of action and therapeutic uses- penicillin, cephalosporins, Quinolones, Aminoglycosides, Carbapenems, macrolide and others. Antibiotic resistance mechanism and implications in therapeutics.

Synthetic studies of : Penicillin V, Streptomycin, Ciprofloxacin

Chemotherapy of Tuberculosis: First line Drugs and second line drugs- chemistry Pharmacology. The problem of MDR tuberculosis.

Antimalarials : Chemotherapy of Malaria, mode of action of the various classes of drugs used, Chemistry, SAR and Drug resistance. Study of the following drugs in the treatment , efficacy , problem of side effects- Qunine sulphate, Chloroquine and proguanil.

Unit 5: Analgesics, Antipyretic & Anti-inflammatory drugs **14 Hours**

Mechanism of action

Different types of analgesics

Narcotic analgesics - morphine and codeine, phenyl (ethyl) piperidines

Antipyretics and NSAIDs: Basic idea of COX I & II inhibitors, salicylates - aspirin, p- aminophenol derivatives-paracetamol, phenacetin, anthranilic acid derivatives – flufenamic acid, arylacetic /propionic acid derivatives (ibuprofen, ketoprofen and diclofenac

Anti-inflammatory: Sulindac, Naproxen

Novel Analgesics: Raxatrigine (Structure only).

Synthesis of the following drugs- pethidine, phenyl butazone, diclofenac, Codeine.

References

1. Medicinal chemistry, S. S. Pandeya and J. R. Dimmock, New Age International
2. G. Patrick, Medicinal Chemistry, BIOS. 2001.
3. T. Nogrady, D.F. Weaver, Medicinal Chemistry, Oxford University Press, 2005.
4. W.O. Foye, T.L. Lemke, D.A. Williams, Principles of Medicinal Chemistry, 4thEdn., Williams & Wilkins, 1995.
5. J.P. Remington, Remington's Pharmaceutical Sciences, Vol.13, , 19th Edn., Mack,1990.
6. D. Sriram , P. Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.
7. K. D. Tripathi, Essentials of Medical Pharmacology, 6th Edn.,Jaypee, 2008
8. L.S. Goodman, A. Gillman, The Pharmacological Basis of Therapeutics, 10thEdn., McGraw Hill, 2001.
9. S.S. Kadam, Principles of Medicinal Chemistry, Vol.I& II, Pragati Books, 2008.
10. Kar, Medicinal Chemistry, New Age International, 2007.
11. C.O. Wilson, J.M. Beale, J.H. Block, Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th Edn., Lippincott Williams and Wilkins, 2010

SEMESTER III

ELECTIVE PAPER II

CHD3E.04 - BIOCHEMISTRY AND BIOPHYSICAL CHEMISTRY

TOTAL HOURS: 72

Unit: I. Amino Acids and Proteins **14 Hours**

Structural and functional classification of proteins. Structure.

Physicochemical properties, configuration and optional properties of amino acids. Purification of proteins and amino acids, sequence determination.

Primary, Secondary Tertiary and Quaternary structure of Proteins.

Protein folding, three dimensional structure of proteins.

Solid phase peptide synthesis.

Unit: II Enzymes **20 Hours**

Enzymes; Classification, Mechanism of enzymatic reactions, kinetics of enzymatic reactions, Michaelis Menton model, Significance of Kmax and Vmax. Inhibition of enzymatic reactions. Kinetics of competitive and non-competitive Inhibition. Allosteric enzymes, Mechanism of enzymatic catalysis by Lysozyme and carboxy peptidase, Zymogens.

Coenzymes; Classification, Structure and Function of Nicotinamide adenine dinucleotides (NAD and NADP), Riboflavin Nucleotides (FMN and FAD), Biological oxidation and reduction, Lipoic acid, Cytochromes, Pyridoxal phosphate, Nucleoside diphosphates. Tetrahydrofolic acid conjugates, Biotinyl coenzyme. Coenzyme - A, and Thiamine pyrophosphate.

Biotechnological Application of Enzymes; Large scale production and purification of enzymes, Techniques and method of immobilization of enzymes, effect of immobilization on enzyme activity, Application of immobilized enzymes, use of enzymes as targets for drug design.

Unit: III Nucleic Acids and Hormones **14 Hours**

Nucleic acids: Nucleic acid bases, Nucleosides, nucleotides, structure of DNA, RNA and its classification.

Replication of DNA, transcription, translation and Protein Biosynthesis.

Restriction enzymes. DNA finger printing Techniques, Introduction to Recombinant DNA technology.

Genetic code, gene therapy (basic concept only), PCR.

Chemical Synthesis of Nucleotides, Restriction enzymes. Chemistry of ATP, ADP and AMP.

Hormones: Functions and mode of action of hormones, Pituitary, thyroid, parathyroid, adrenal and adrenocorticoid and pancreatic hormones. Male and female sex hormones. Anti-hormones.

Unit V Biological oxidation and metabolism: 14 Hours

Carbohydrate metabolism-Carbohydrate the source of energy, glycolysis, glycogenesis, pentose pathway, citric acid and Cori cycle.

Regulation of carbohydrate metabolism, Hormonal regulation of carbohydrate metabolism. Fructose and Galactose metabolism.

Diabetes- Type I &II.

Lipid metabolism: Oxidation of fatty acid, biosynthesis of fatty acids, Prostaglandins-classification , structure and biosynthesis and biological role.

Protein and amino acid metabolism: Oxidative deamination and trans amination reactions, Urea formation- ornithine cycle.

UNIT VII: Buffer systems 10 Hours

Biological relevance of pH and pKa, determination of pKa of weak acid

Buffer in pharmaceutical and biological systems, pH, the buffer equation (Henderson Hesselbach), Buffer calculations. Three important buffer systems in human body (cytosol and blood). Buffer capacity, osmotic pressure and tonicity, Pharmaceutical buffers, preparations of pharmaceutical buffer solutions.

References

1. Lehninger- Principles of Biochemistry; DL Nelson and MM Cox, 6th Edn. Macmillan Publications (2012).
2. Biochemistry VI Edition; Jeremy M Berg, John L Tymoczko and Lubert Stryer, W H Freeman and Co. (2006).
3. Physical Biology of the Cell, 2nd Edn. Rob Phillips, Jane Kondev, Julie Theriot, Hernan Garcia, Garland Publishers (2012).
4. Biochemistry; Voet, D. and Voet, J.G. [Eds.] 3rd Ed. Jhon Wiley and sons, (1999).
5. Biochemistry; David Rawn, J, Neil Patterson Publishers (1989).
6. Complex Carbohydrates, Sharon, N. Addison Wisely, (1975).
7. Methods of Enzymatic Analysis; Berg Meyer Vol. 1-X, (1974). 10
8. Nucleic acid Biochemistry and Molecular Biology, Mainwaring et al., Blackwell Scientific (1982).
9. Principles of Biochemistry; Smith et al., McGarw Hill (1986).
10. Proteins Structures and Molecular Properties 2nd Edn. Thomas E. Creighton, W H Freeman and Co. (1993).
11. Principles of Protein Structure, Function, & evolution, Dickerson & Geis 2nd Ed. Benjamin-Cummings (1983).
12. Biochemistry Ed. Donald Voet & Judith G. Voet, John Wiley & Sons, Inc.(2010).
13. Practical Biostatistics; Mendel Suchmacher and Mauro Geller, Academic Press (2012).

14. Sadasivan S & Manikam A, Biochemical methods. New Age International.
15. Chatterji M N & Rana Shindo, Text Book of Medical Biochemistry. J P Brothers.
16. DasDebjyoti,Biochemistry.AcademicPublishers.

SEMESTER – III

CHD3C.08 - INORGANIC CHEMISTRY – II

TOTAL HOURS: 72

UNIT – I **18 HOURS**

COORDINATION CHEMISTRY – I

Coordination numbers 2 to 12 and geometry – VB theory, assumption and limitations. Crystal field theory of coordination compounds – d-orbital splitting in octahedral, tetrahedral and square planar fields. Crystal field effect on ionic radii and lattice energies – Jahn teller effect – evidence for ligand field splitting – spectrochemical series.

MOT in coordination compounds – MO energy level diagrams for octahedral, tetrahedral and square planar configuration with and without π bonding. Effect of π bonding in stability – nephelauxetic series – experimental evidence for metal-ligand. Covalent bonding in complex. Comparison of three theories as applied to metal complexes.

UNIT – II **18 HOURS**

COORDINATION CHEMISTRY – II

Spectroscopic ground states – term symbols for d^n ion. selection rules for d-d transitions – nature of spectral bands – (band shapes, intensities, width and spin orbit coupling) Orgel diagram of transition metal complexes(d^1 to d^9 configurations) Tanabe Sugano diagrams, interpretation of spectra of spin paired and spin free octahedral, distorted octahedral, tetrahedral and square planar complexes. Magnetic behaviors – susceptibility, measurements – Gouy method diamagnetic corrections. Spin only value – orbital contributions – spin orbit coupling, ferro and antiferro magnetic coupling – spin cross over system – Applications of magnetic measurements to structural determinations of transition metal complexes.

UNIT – III **18 HOURS**

COORDINATION CHEMISTRY III

Reaction of complexes: Ligand substitution reactions (Square planar and octahedral complexes). Rates of ligand substitutions, classification of mechanisms. Nucleophilicity of the entering group, The shape of the transition states, The activation of octahedral complexes, Base hydrolysis, stereochemistry, Isomerisation reactions. Brief study of redox reaction and photochemical reactions.

Reaction of metal complexes: Stability constants – chelate effect – Irving-William order of stability. Factors affecting the stability of metal complexes. Determination of binary formation constants by pH meter and spectrophotometry- energy profile of a reaction.

UNIT–IV **18HOURS**

ORGANOMETALLIC CHEMISTRY

Introduction: General methods of preparations – General properties – organometallic compounds of alkali metals, organometallic compounds of beryllium – organometallic compounds of Mg, Al. Metal-olefin (alkene) complexes. Transition metal alkyls and aryls and

their applications d- block carbonyls.
Metallocenes, metal-metal bonding and metal clusters. Reactions – oxidative addition and reductive elimination. σ-bond meta thesis. 1 + 1 migratory insertion reactions. Catalysis by organometallic compounds (eg: alkene hydrogenation, hydroformylation, Monsanto acetic acid process)

REFERENCE

1) S F A Kettle, Coordination Chemistry, Thomas Nelson and Sons
2) J C Bailer, Chemistry of coordination compounds, Reinhold
3) F Basolo R Johnson, Coordination Chemistry, Benjamin Inc
4) D Banergea, Coordination Chemistry, Tata McGraw Hill
5) D N Sathyanarayana, Electronic Absorption spectroscopy and related techniques, Universities Press
6) R Gopala and V N Ramalingam, Concise Coordination Chemistry, Vikas publishing house Pvt Ltd
7) M C Day and J Selbin, Theoretical Inorganic Chemistry, Affiliated EAST West Press
8) J E Huhee, Inorganic chemistry principles of structure and reactivity, Pearson Education India
9) R L Dutta and A Syamal, Elements of magneto chemistry, S Chand and Company Ltd
10) Glen E Rodgers, Inorganic and solid state chemistry, Ceengage Learning
11) Indrajith Kumar, Organometallic compounds, Pragati Prakashan Meerut
12) R C Melhtra and A Singh, Organometallic Chemistry, New age international

SEMESTER – III

CHD3C.09 - ORGANIC CHEMISTRY – III

TOTAL HOURS: 72

UNIT – I **18 HOURS**

ELECTRONIC AND IR SPECTROSCOPY

Colour and light absorption – the chromophore concepts – theory of electronic spectroscopy – laws of light absorption – Beer-Lamberts law – solvents and solutions – effect of solvent polarity on UV absorption – electronic transition in enes, enones and arenes, Woodward Fischer rule – instrumentation and sampling

IR spectroscopy – factors influencing vibrational frequencies – principles of characteristics frequency in IR- application of IR – identity by finger printing – identification of functional groups and other structural features by IR – Hydrogen bonding and IR bands – Instrumentation and sampling techniques – FTIR and its instrumentation

UNIT – II **18 HOURS**

NMR SPECTROSCOPY

Chemical shifts – anisotropic effect and coupling constants in organic compounds, spin-spin interaction in typical systems – analysis of 1^{st} order spectra - simplification methods for complex spectra – use of high field NMR – shift reagents, chemical exchange and double resonance – introduction to FT(PULSE) NMR, NOE, DEPT and 2D NMR, C13 NMR and C13 chemical shift – structural applications of C13 NMR – spectral interpretation and structure identification – spectral interpretation using actual spectra taken from standard texts – solving of structural problems on the basis of numerical and spectral based data – NMR spectroscopy of N, F and P (qualitative) – chemically induced dynamic nuclear polarization (CIDNP)

UNIT – III **18 HOURS**

ORGANIC MASS SPECTROSCOPY

Instrumentation – EI, CA, FAB, Electro spray and MALDI ion sources – magnetic high resolution (double focusing), TOF and Quadrupole mass analyzers – isotope abundance - molecular ion – molecular mass from molecular ion – meta stable ion – significance of meta stable ion – fragmentation process – basic fragmentation types and rule – factors influencing fragmentation – fragmentation associated with functional groups – alkanes, alkyne, halides, alcohols, ethers, carbonyl compounds, carboxylic acids, amides – characteristic fragmentation modes and Mc Lafferty rearrangement – GC-MS, HPLC-MS, TG-MS. Structural elucidation of organic compounds based on UV, IR, NMR, and MS data

UNIT – IV **18 HOURS**

HETEROCYCLIC CHEMISTRY

Nomenclature of heterocycles, replacement and systematic nomenclature, Hantzsch-Widman system for monocyclic fused and bridged hetero cycles. Structure reactivity, synthesis and

reactions of the following four membered heterocycles – oxitanes, azetidines and thietanes; five membered heterocylces – imidazoles, pyrazolines, 1,2,4 – triazoles, 1,2,3 –triazoles, oxadiazole and thiadiazole; selenophenes, tellurophanes and their benzoderivatives; six membered heterocycles – pyrans, 1,2,3-, 1,2,4- and 1,2,5-triazines, pyrimidines and pyrazines; seven membered heterocyles – azepines, oxepines and thiepines – fused heterocycles; indole, benzofuran, quinoline, isoquinoline and coumarins. Naphthyridines – synthesis and reactivities

REFERENCES

1. W Kemp, Organic spectroscopy, Palgrave
2. J March, Advanced organic chemistry, Wiley
3. R O C Norman and A Coxon, Modern synthetic reaction, Chapman and Hill
4. M B Smith, Organic synthesis, McGraw Hill
5. R K Bansal, Synthetic applications in organic chemistry, Narosa
6. Robert M Silverstein, Francis X. Webster and David Kiemle, Spectrometric identification of organic compounds, Wiley 2005
7. Donald L Pavia, Gary M Lampman, George S Kriz and James R Vyvyan, Spectroscopy, Cengage Learning
8. RATAN Kumar Kar, Applications of redox and reagents in organic synthesis, New Central Book Agency
9. J Jouly and G Smith, Heterocyclic chemistry, Van-Nostrand, ELBS
10. Acheson, An introductory to heterocyclic compounds, Wiley-Eastern
11. Ahluwalia and Parashar, Heterocyclic and carbocyclic chemistry, Ane Books
12. Jagadamba Singh and Yadav, Organic synthesis, Pragati Prakashan Meerut
13. S K gosh, Advance general Organic chemistry part 1 and 11, New central book agency

SEMESTER – III

CHD3C.10 - PHYSICAL CHEMISTRY – III

TOTAL HOURS: 72

UNIT – I **18 HOURS**

REACTION KINETICS

Review of basic principles: Complex reactions- Reversible, para**l**lel, consecutive and branching reactions- Principles of microscopic reversibility. Theories of reaction rate- collision theory– steric factor-potential energy surfaces- transition state theory- Eyring equation- comparison of two theories-Thermodynamic formulation of reaction rates- significance of $\Delta G^{\#}$, $\Delta H^{\#}$ and $\Delta S^{\#}$ volume of activation- Effect of pressure and volume on the velocity gas reaction–Unimolecular reaction- Lindmann, Hinshelwood mechanism and RRK theories- Fast reaction–relaxation, flow method-flash photolysis –Magnetic and Resonance method. Theoretical calculation of energy of activation.

UNIT – II **18 HOURS**

KINETICS AND CATALYSIS

Chain reaction–stationary and non-stationary chain- explosion and explosion limits-free radical and chain reaction- steady state treatment- kinetics of H_2-CI_2 and H_2-Br_2 - decomposition of acetaldehyde- Rice Herzfeld mechanism- Branching chain-H_2O_2 reaction-Semenov Hinshelwood mechanism of explosive reaction.

Acid – base catalysis-specific and general catalysis-prototropic and protolytic mechanism-examples-Acidity function. Enzyme catalysis-Michaelis-Menten equation- derivation-effect of pH and temperature. Reaction in solution- Factors determining reaction rates in solution–Effect of pressure-dielectric constant-ionic strength-cage effect-Bronsted- Bjerrum equation-Primary and secondary kinetic salt effect-Influence of solvent on reaction rate- Hammet & Taft equation.

UNIT – III **18 HOURS**

SURFACE CHEMISTRY

Different types of surfaces – Thermodynamics of surfaces –Gibbs adsorption equation and its verification -surfactants and micelles – surface film- surface pressure and surface potential and their measurements - interpretation- Application of Low energy electron- Diffraction and photoelectron spectroscopy- ESCA and Auger Spectroscopy to the study of surfaces. Adsorption-Langmuir adsorption isotherm - Different types- BET theory and Harkins – Jura theory– Measurement of surface area of solids using Langmuir, BET and Harkins-Jura isotherm-Heat of adsorption- adsorption- isosters and determination of heat of adsorption-Langmuir adsorption isotherm applied to rate laws for surface catalyzed reaction- The Eley Rideal mechanism – flash desorption.

UNIT – IV **18 HOURS**

COLLOIDS

Structure and stability of colloids, Micelles– The electrical double layer-Electro kinetic phenomena-zeta potential-electro osmosis- colloids-zeta potential(derivation)-sedimentation potential- streaming potential- Donnan membrane equilibrium-Macro molecules-different averages-Methods of molecular mass determination–Osmotic method- sedimentation methods-light scattering methods. Macromolecular dynamics, diffusion coefficient – diffusion coefficients and molecular size, sedimentation coefficient - electrophoresis

REFERENCES

1. K.J.Laidler -"*Chemical kinetics*" Pearson Education
2. S.Glasstone, K.J. Laidler and Eyring-"*The Theory of rate processes*"- McGraw Hills
3. J. Rajaram and J.C. Kuriacose- "*Kinetics and Mechanism of chemical transformations*"- MacMilan India Ltd
4. Alberty and Silbey-"*Physical chemistry*"-Wiley
5. G.K.Vemulappally-"*Physical chemistry*"-Prentice Hall of India
6. P.W.Atkins-"*Physical chemistry*"-Oxford University press
7. A.W.Adamson-"*The physical chemistry of surfaces*"- 4th edition-Wiley1982
8. Alexander and Johnson-"*Colloid science*"-Oxford University Press
9. Gowariker-"*Polymer science*"–New age International publishers
10. K.J.Laidler-John.H.Melser-"*Physical chemistry*"-CBS
11. Gorgen M Barrow, "*Physical Chemistry*", 5th edn Tata McGraw-Hill

SEMESTER IV

ELECTIVE PAPER III

CHD4E.05 - DRUG CHEMISTRY AND DRUG DESIGN

TOTAL HOURS: 72

UNIT 1. Drug Design and Development **12 Hours**

Development of new drugs, procedures followed in drug design - Concept of lead compounds and lead modification & lead optimization- phytochemicals as lead compounds - Prodrugs and soft drugs. Functions and properties of prodrugs and its effect and significance with relation to pharmacological activity - Endogenous compounds as drugs -neurotransmitters, natural hormones - Peptidomemetics in drug design - SAR, factors affecting bioavailability, resonance and inductive effects, isosterism, bioisosterism – thermodynamics of biological systems.

UNIT 2. Computer Aided Drug Design (CADD) **12 Hours**

Virtual screening- concept, drug likeness screening, focused screening libraries for lead identification, pharmacophore screening, and structure based virtual screening and application.

Molecular modeling- introduction, molecular methods, Molecular mechanics, modeling ligands for known and unknown receptors. Docking studies - Machine Learning Approaches to Rational Drug Design

UNIT 2. QSAR **10 Hours**

Introduction and perspectives and parameters involved in studies of QSAR - Types of QSAR models - Classification of parameters utilized in QSAR studies - Statistical concept of QSAR - Hansch model of QSAR - De Novo model of QSAR - Hammett and Taft model of QSAR equations - Applications of QSAR in drug design

UNIT 4. Combinatorial Chemistry **10 Hours**

Introduction - Combinatorial approaches - Peptide and small molecule libraries - Applications, methodology - Combinatorial Organic Synthesis - Assays and Screening of Combinatorial libraries - Introduction to High Throughputs Screening (HTS)

UNIT 6. Antineoplastic drugs **10 Hours**

Cancer chemotherapy - Role of alkylating agents, antimetabolites and folate antagonists in the treatment of cancer. Carcinolytic antibiotics and mitotic inhibitors - Plant derived drugs - vincristine, taxol - Hormones and their antagonists - Recent developments in cancer chemotherapy - immunological interventions.

UNIT 7. Drugs acting on ANS **10 Hours**

Introduction to autonomic nervous system and classification. Mechanism of action and uses of the following classes of drugs: Adrenergic agonists : oxymetazoline, salbutamol. Adrenergic blockers: α and β adreno-receptors, antagonists-ergot alkaloids- Pronethalol, propranolol, atenolol. Cholinergic stimulants: nicotinic and muscarinic receptors, acetyl choline. Cholinergic blockers: atropine. Nicotinic antagonists: Decamethonium and suxamethonium. Organo phosphorous compounds and nerve gases (Elementary idea only).

UNIT 8. Drugs acting on Central Nervous System **8 hours**

Pharmacology of the following classes of drugs

Hypnotics, sedatives and anxiolytic agents.
Anxiolytic agents-benzodiazepines, buspirone and meprobamate.
Anticonvulsants: Barbiturates- hydantoins, oxazolidinediones, succinimides and benzodiazepines.
Analeptics: xanthines, amphetamines, nikethamide and ethamivan.
Centrally acting muscle relaxants: glyceryl ethers-mephenesin, alkane diol derivatives meprobamate, benzodiazepines-librium, diazepam and baclofen.

REFERENCES:

1. Essentials of Pharmaceutical Chemistry, Donald Carins; pharmaceutical Press, 3 Edn.
2. Principles of Medicinal Chemistry, William Foye, Lippincott 5 Edn
3. Text Book of Medicinal and Pharmaceutical Chemistry, Wilson &Gisvold Lippincott, 10 Edn.
4. Medicinal Chemistry & Drug Discovery, Alfred Burger, John Wiley 6 Edn, 2007
5. Fundamentals of Medicinal Chemistry ,G. Thomas. Wiley Publications 2006
6. An Introduction to Medicinal Chemistry, Graham L Patrick, Oxford University Press 2006
7. Organic Chemistry Vol:II, IL FINAR
8. Natural Products Chemistry, NR Krishnaswami, Oxford University Press, 2008
9. Recent Progress in Medicinal Plants Vol.I, Singh, Govil, Tec. Publications LLC, USA,2002.
10. Computer aided Drug design, TJ PERUN7 CL Propst, Marcel& Dekker, 2007.
11. Introduction to Principles of Drug Design, Smith H J, Williams H Edn. Wright Boston
12. Computer Aided Drug Design, Pope & Perruns, Academic Press, NY.
13. Heterocyclic Chemistry in Drug Discovery, Edn, JIE Jack Li, Wiley.
14. Organic Chemistry of Drug Design and Drug Action Richard B Silverman Academic Press
15. Computational Medicinal Chemistry for Drug Discovery, P Bultinck, P DeVinter.
16. Medicinal Chemistry, Alex Gringauz, Wiley India.

SEMESTER IV
ELECTIVE PAPER III

CHD4E.06 - MEDICINAL CHEMISTRY

TOTAL HOURS: 72

UNIT – I — 18 HOURS

a) Introduction: Nature and source of drugs – study of drugs – important terminologies in pharmaceutical chemistry

b) Classification and nomenclature of drugs: biological classification, chemical classification, classification of drugs according to commercial considerate, classification by lay public, nomenclature of drugs, some important heterocyclic systems and their nomenclature

c) Mechanism of drug action and metabolism of drugs: Introduction – mechanism of action of drug, mechanism of different types of drug action, metabolism of drugs, absorption of drugs, assay of drugs

UNIT – II — 18 HOURS

a) Antibacterial drugs: Sulpha drugs; sulphanilamides – properties of sulphanilamides, mechanism of action of sulfa drugs, sulphadiazine, sulphapyridine, cibazole, sulphafurazole, Prontosil – Antibiotics; classification of antibiotics, chloramphenical, pencillin, streptomycin, tetracycline, macrolides

b) Antiseptic and disinfectants: Phenols and its derivatives – halogen compounds –dyes – organic mercurials – formaldehyde and its derivatives – nitrofuran derivatives – cationic surface active agents

UNIT – III

18 HOURS

a) Anesthetics: General anesthetics – volatile general anesthetics; ether, chloroform, haloethane, trichloroethylene, ethyl chloride, nitrous oxide, cyclopropane – Intravenous anesthetics; thiopental sodium, methohexitone – local anesthetics; the esters, cocaine, benzocaine, procaine, amethocaine, proxy metacaine – the amides; lignocaine, cinchocaine

b) Analgesics, antipyretic, and anti-inflammatory agents: Narcotic analgesics – natural narcotic analgesics; morphene, heroin, apomorphine – synthetic narcotic analgesics; pethidine, morphinan, benzomorphan – non narcotic analgesics; salicylic acid derivatives, the paraminophenol, the pyrazole, indolyl and aryl acetic acid derivatives.

UNIT – IV **18 HOURS**

CAUSES OF COMMON DISEASES AND THEIR TREATMENT BY DRUGS

Insect borne disease and their treatment; malaria, filariasis, plague – air borne disease, their controls and treatment; diphtheria, wooping cough, influenza, measles, mumps, tuberculosis – water borne diseases; cholera, typhoid, dysentery –disorders of digestive systems – jaundice – disease of respiratory system; asthma – common disorder of nerve system; epilepsy – some common diseases; piles, leprosy – first aid for accidents – detection of hallucinogens and poisons - antidotes for poisoning

REFERENCES

1. Jayashree Gosh, Fundamental concepts of Applied Chemistry, S Chand
2. K D Tripathi, Essentials of medical pharmacology, 6th edtn, Jaypee
3. G Thomas, Medicinal Chemistry an introduction, Wiley
4. G L Patrick, Introduction to Medicinal Chemistry, Oxford
5. A Kar, Medicinal chemistry, New age
6. D Sriram, P Yogeeswari, Medicinal Chemistry, Pearson Education
7. G Thomas, Fundamentals of Medicinal Chemistry, Wiley

SEMESTER – IV

CHD4C.11 - INORGANIC CHEMISTRY – III

TOTAL HOURS: 72

UNIT – I **18 HOURS**

PHYSICAL TECHNIQUES IN INORGANIC CHEMISTRY

Study of inorganic compounds by the following methods Diffraction methods – X-ray diffraction, neutron diffraction
Absorption spectroscopy – UV Spectroscopy, Infra red and Raman spectroscopy

Resonance technique – nuclear magnetic resonance, electron para magnetic resonance, mossbaur spectroscopy
Ionization base techniques – photon electron spectroscopy, x-ray absorption spectroscopy, mass spectrometry
Chemical analysis – atomic absorption spectroscopy, CHN Analysis, X-ray fluorescence elemental analysis
Thermal analysis

Magnetometry – electrochemical techniques

UNIT – II **18 HOURS**

METALLURGY AND CHEMISTRY OF F BLOCK ELEMENTS

Thermodynamic aspects of extraction. Ellingham diagrams – Latimer Frost diagrams. Extraction properties and uses of thorium, uranium, and plutonium.
Beach sands of Kerala – important components and their separation from-monazite, illuminite, zircon, and sillimanite

Lanthanides:- electronic structure, oxidation states – chemical properties of +2,+3 and +4 oxidation state – lanthanide contraction – spectral and magnetic properties. Coordination number and stereochemistry of complexes

Actinides:- electronic structure – oxidation states – actinide contraction – spectral and magnetic properties in comparison with those of lanthanides and d-block elements. Trans actinide elements, IUPAC nomenclature – periodicity of trans actinide elements.

UNIT – III **18 HOURS**

BIO INORGANIC CHEMISTRY

The organization of cell – physical structure of cells, the inorganic composition of cells. Role of metal ions in the biological system. Essential and non essential elements.
Transport, transfer and transcription – sodium and potassium transport, calcium signaling proteins, zinc in transcription, selective transport and storage of iron, oxygen transport and storage, electron transfer.
Biological cycles – nitrogen cycle, hydrogen cycle

Sensors – iron proteins as sensors, proteins that sense copper and zinc levels. Biomineralization Chemistry of elements in medicine – chelation therapy, cancer treatment, antiathrities drugs, imaging agents

UNIT – IV **18 HOURS**

TRANSITION METAL CARBONYLS AND RELATED COMPOUNDS

Introduction – preparation and properties of transition metal carbonyls – structures of transition metal carbonyl, structures of some carbonyls like $Ni(CO)_4$, $Fe(CO)_5$, $Cr(CO)_6$, $Fe_2(CO)_9$, $Co_2(CO)_8$, $Mn_2(CO)_{10}$, $Tc_2(CO)_{10}$, $Re_2(CO)_{10}$, $Fe_3(CO)_{12}$ and $Os_3(CO)_{12}$ and calculation of EAN of metal atom – carbonyl hydrides and carbonylate anions and cations – carbonyl halides – phosphene and phosphorous trihalides complexes. Dinitrogen complexes – nitric oxide complexes – cyano complexes

REFERENCE

1. Alan G Sharp – Inorganic chemistry third edition, Pearson
2. J E Huheey, E A Keiter and R L Keiter, Inorganic chemistry principles of structure and reactivity, Pearson education
3. D F Shriver and P W Atkins, Inorganic Chemistry, Oxford University Press
4. Sathya prakash, G D Tuli, S K Basu and R D Madan, Advanced inorganic chemistry Volume II, S Chand Publication
5. Cotton, Wilkinson, Bachmann, Advanced inorganic chemistry, Wiley India Pvt Ltd
6. B Douglas D McDaniel and J Alexander, Concepts and models of inorganic chemistry 3rd edition, John Wiley and Sons Inc
7. S J Lippard and J M Berg, Principles of bioinorganic chemistry, University Books California
8. David E Fenton, Bio coordination chemistry, Oxford University Press
9. I Bertni, H B Grey, S J Lippard and J S Valentine, Bio inorganic chemistry, Viva Books Pvt Ltd, New Delhi
10. DMP Mingo's Essential Trends in inorganic chemistry, Oxford University Press
11. K Hussain Reddy Bioinorganic chemistry New age international

SEMESTER IV

CHD4C.12 - INTER DISCIPLINARY TOPICS AND INSTRUMENTATION TECHNIQUES

TOTAL HOURS: 72

UNIT – I **18 HOURS**

SUPRA MOLECULAR CHEMISTRY

Introduction to supra molecular chemistry, molecular forces, common supra molecules, experimental techniques in supra molecular chemistry, host/guest chemistry, molecular recognition – molecular receptors for different types of molecules including arisonic substrates, design and synthesis of co receptor molecule and multiple recognition – amphiphile organization, supra molecular design strategy and nanotechnology. Supra molecular devices. Supra molecular photochemistry, supra molecular electronic, ionic and switching devices.

UNIT – II **18 HOURS**

GREEN CHEMISTRY

Introduction, the need of green chemistry, principles of green chemistry, plaining of green synthesis, tools of green chemistry, green reactions, Aldol condensation, Cannizaro reaction and Grignard reaction – comparison of above with classical reactions – green preparations, applications – phase transfer catalyst – introduction to microwave organic synthesis – applications: environmental, solvents, time and energy benefits

UNIT – III **18 HOURS**

NANOSCIENCE AND TECHNOLOGY

Introduction – nanostructures,: tubes, fibers, bricks and building block, nanostructure formation: lithography, self-assembly, molecular synthesis, crystal growth and polymerization, measurement of nanostructure: spectroscopy, microscopy and electrochemistry, nano CAD, material study: nano composites, consumer goods, smart materials, applications to various fields: optics, telecommunication, electronic, digital technology, and environmental, biomedical applications; diagnosation, protic engineering, mapping of genes, drug delivery, biomimetics, quantum dots

UNIT – IV **18 HOURS**

INSTRUMENTATION TECHNIQUES

Principles, instrumentation and application of thermogravimetry, differential thermal analysis, differential scanning calorimetry, dynamic mechanical analyzer, thermo chemical analyzer, direct injection enthalpymetry and thermometric titrimetry.

Scattering methods – Nephelometry and turbidimetry – effects of concentration, particle size and wavelength of scattering, instrumentation and application.

Electron spin resonance spectroscopy – basic principles – hyperfine coupling – the g values – isotropic and anisotrpic hyperfine coupling constants – zero field splitting and kramers degeneracy – application to simple inorganic and organic free radicals and to inorganic complexes

Mossbauer spectroscopy; The Mossbauer effect – chemical isomer shift – Doppler effect – quadrupole interactions – measurement techniques and spectrum display – application to the study of Fe^{2+} and Fe^{3+}

REFERENCE

1. V K Alhuvalia, Green Chemistry, Ane books
2. P T Anastas and J C Warner Green Chemistry Oxford
3. G A Ozin, A C Arsenault, Nano chemistry RSC
4. Diwan, Bharadwaj, Nano composites, Pentagon
5. V S Muralidharan, A Subramania, Nano science and technology, Ane books
6. Willard Merit, Dean, Kettle, Instrumental methods of analysis, 7th ed CBS.
7. Chatwal- Anand, Instrumental analysis of chemical analysis, Himalaya publishing house

CHD3&4P.04 INORGANIC CHEMISTRY PRACTICAL – II

(3rd and 4th SEMESTER)

TIME: 108 HOURS

Credit 2

1) Quantitative separation of binary mixtures and estimation of components by volumetric, gravimetric, colorimetric and electroanalytical methods
   Cu(II), Ni(II), Fe(III), Mg(II), Al(III), Ca(II), Ba(II) and Zn(II)
2) Analysis of ores and alloys
   a) Analysis of dolomite – Insoluble residue by gravimetric and Ca and Mg by complexometry
   b) Pyrolusite – Insoluble residue by gravimetric and MnO_2 by permanganometry
   c) Analysis of brass
   d) Analysis of solder – Pb and Sn by EDTA method
3) Ion exchange separation of binary mixtures such as those of Zn(II), Mg(II) and Co(II), Ni(II)
4) Preparation of following complexes and checking the purity by metal content analysis
   a) Potassiumtrioxalatoferrate(II)
   b) Potassiumhexathiocyanatochromate(III)

REFERENCE

1) G H Jeffrey, J Bassette, J Mendham and R C Denny, Vogel's text book of quantitative inorganic analysis, ELBS Publication, London 1997
2) D M Adams and J B Raynor, Advanced practical inorganic chemistry, CRC Press, New York
3) W L Jolly, Preparative Inorganic reactions, Interscience publishers, New York

CHD3&4P.05 ORGANIC CHEMISTRY PRACTICAL – II

(3rd and 4th semester)

TIME: 108 HOURS

Credit 2

(A minimum of 20 experiments to be done)

1. Quantitative analysis: Determination of
   a) Equivalent weight of a carboxylic acid, b) Reducing sugars using Fehling solution,
   c) Phenol, salicylic acid, aspirin and aniline using bromated bromide mixture, d) keto methyl group in water soluble ketones such as MEK and acetone,
   e) Iodine and saponification of vegetable oil f) nitrogen by Kjeldahl method and sulfur gravimetrically and g) colorimetric estimation of ascorbic acid
2. Preparation of the following organic compounds by the indicated routes
   a) p-nitroaniline: acetanilide- p-nitroacetanilide -p-nitroaniline
   b) 1,3,5-tribromobenzene: aniline -1,3,5-tribormoaniline -1,3,5-tribromobenzene
   c) Methyl orange: Aniline sulphanilic acid methyle oragnge
   d) p-aminoazobenzene: aniline diazoaminobenzene p-aminoazobenzene
   e) N-acetylanthranilic acid: o-toluedine -o-methylacetanilide N-acetylanthranilic acid
   f) p-chlorobenzoic acid: p-toluedine -p-chlorotoluene p-chlorobenzoic acid
   g) m-nitroaniline: nitrobenzene m-dinitrobenzene m-nitroaniline
   h) Benzyl: benzaldehyde benzoin benzyl
   i) m-nitrobenzoic acid: methylbenzoate—m-nitromethylbenzoate -m-nitrobenzoic acid
   j) Benzanilide: benzophenone benzophenone oxime—benzanilide
3. Extraction of natural products: Caffeine from tea leaves, chlorophyll (Soxhlet extraction), citral from lemon grass (steam distillation), casein from milk
4. Practical application of TLC: Identification of food colours, aminoacids, sugars, terpenoids, alkaloids, steroids, flavanoids, organo chloro pesticides, organo phosphorus pesticides, organo phosphours pesticides, carbamate pesticide, indole acetic acid
5. Synthesis of some typical organic medicinal compounds, spectral illustration of the intermediates and products formed: paracetamol, sulphanilamide, hippuran, benzocaine, clofibrate, mercurochrome, phenytoin, dapsone, sulphasalazine, antipyrine, aminacrine and phenobarbitone.
6. Preparation of some specified crude plant extracts and qualitative analysis by TLC of crude plant extracts/ products to detect the presence of phytochemicals
7. Isolation of phytochemicals from their natural sources:
   Examples: Caffeine from Tea, Nicotine from tobacco, Curcumin from turmeric, Tannins from Gallnuts, Lycopene from tomato etc.
8. Qualitative analysis of barbiturates, lactates, tartrates and alkaloids
9. Assay of Antibiotics.
10. Assay of Vitamins: ascorbic acid, acetomenaphthone, niacinamide, pyridoxine and thiamine.

REFERENCE

1. A I Vogel, A Textbook of Practical Organic Chemistry, Longman
2. Elementary Practical Organic Chemistry, part 3, quantitative organic analysis Longman
3. F G Mann and B C Saunders, Practical Organic Chemistry, Longman
4. P R Singh, D C Gupta and K S Bajpal, Experimental Organic Chemistry vol I and II
5. S Sadasivam and A Manickam, Biochemical methods, New age International Publishers
6. J B Harbone, Phytochemical methods, Chapman and Hall, London
7. Joseph Sharma, Gunter Zweig, TLC and LC Analysis of international importance, Vol. VI and VII, Academic Press

CHD3&4P.06 PHYSICAL CHEMISTRY PRACTICAL – II

(3rd and 4th SEMESTER)

TIME: 108 HOURS

Credit 2

A minimum of 20 experiments covering all units

Chemical kinetics experiments

1. Acid hydrolysis of ester (methyl acetate or ethyl acetate) – determination of the given acids.
2. Acid Hydrolysis of ester – determination of Arrhenius parameters
3. Saponification of ethyl acetate – determination of specific reaction rate, K2S2O8 and KI system
4. Iodination of acetone in acid medium – determination of order of reaction with respect to iodine and acetone

Adsorption experiments

1. Verification of Freundlich and Langmuir adsorption isotherms – charcoal-acetic acid system
2. Determination of concentration of given acetic acid solution using the isotherms
3. Same experiment using charcoal-oxalic acid system

Conductivity experiments

1. Equivalent conductance of weak acids – verification of Ostwald's dilution law – calculation of dissociation constant
2. Equivalent conductance of strong electrolytes (KCl). Verification of Onsagar equation
3. Activity coefficient of zinc in 0.002 M $ZnSO_4$ using Debye-Huckel limiting law
4. Solubility product of sparingly soluble salts (AgCl-$BaSO_4$)
5. Conductance titrations. HCl vs NaOH, (HCl+HOAc) vs NaOH, $AgNO_3$ vs KCl

Polarimetry Experiments

1. Determination of specific and molar optical rotations of glucose, fructose and sucrose
2. Determination of the concentration of a glucose solution
3. Inversion of cane sugar in presence of HCl-Study of the kinetics
4. Determination of specific rate of the reaction
5. Determination of the concentration of HCl

Spectrophotometry Experiments

1. Verification of the Beer Lamberts law
2. Determination of equilibrium constants of acid-base indicators
3. Determination of concentration of a solution of $K_2Cr_2O_7$ (or $KMnO_4$)
4. Simultaneous determination of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$
5. Investigation of complex formation between Fe(III) and thiocyanate

Computational & Drug Chemistry Experiments (Any four experiments)

1. Geometry optimization and single point energy calculations of simple organic molecules
2. Calculation of energy gap between HOMO and LUMO in simple molecules and visualization of molecular orbitals
3. Calculation of dipole moment in polar organic molecules.
4. Calculation of electrostatic charges of atoms in organic molecules using population analysis

5. Calculation of Resonance energy of aromatic compounds
6. Prediction of the stability of ortho, meta, para products of nitration of aromatic ring using computational chemistry calculations.
7. Calculation of IR stretching frequencies of groups and visualization of normal modes of vibration in organic molecules.
8. Calculation of dimerization energy of carboxylic acids
9. Perform the conformational analysis of butane using potential energy scan
10. Find the transition state of simple organic reactions and plot the reaction profile.
11. Determination of heat of hydration of organic molecules.
12. Find the Gibbs free energy of simple gaseous phase reactions and calculate equilibrium constant.
13. Spectral analysis (UV, IR and NMR) of simple organic molecules.
14. Perform molecular dynamic simulations of smaller molecules in water.
15. Calculation of p^{ka} of simple organic molecules and compare it with experimental values
16. Docking studies involving protein ligand interactions.
17. Calculation of electrophilicity index in hard-soft acids and bases.

REFERENCES

1. F Danieles and J H Mathews, Experimental physical chemistry, Longmann
2. A M James, Practical physical chemistry, J A Churchill
3. H H Williard, L L Merit and J A Dean, Instrumental methods of analysis, Affiliated
1. East West Press
4. D P Shoemaker and C W Garland, Experimental physical chemistry, McGraw Hill
5. J B Yadav, Advanced practical physical chemistry, Goel Publishers
6. B Viswanathan, P S Raghavan, Practical physical chemistry, Viva Books Pvt Ltd
7. V D Athawale Parul Mathur, Experimental physical chemistry, New age International Publishers
8. A Findlay and J A Kitchener, Practical physical chemistry, Longmann

MODEL QUESTION PAPER

(Common in all theory papers and elective papers) Sample 1
CHD1C.03 - ORGANIC CHEMISTRY – I

Time: 3 Hours **Max Marks: 60**

Section A

Answer all questions in one word or one sentence. Each question carries one mark

1.

2.

3.

4.

5.

6.

7.

8.

(8 X 1 =8 marks)

Section B

Answer any eight questions. Answer may be two or three sentences. Each question carries two marks

9.

10.

11.

12.

13.

14.

15.

16.

17.

18.

19.

20.

(8 X 2 = 16marks)

Section C

Short paragraph questions. Answer any four questions. Each question carries 3 marks

21.

22.

23.

24.

25.

26.

27.

28.

(4 X 3 = 12marks)

Section D

Essay type questions. Answer four questions. Each question carries 6 marks.

27. A.

Or

B.

28. A.

Or

B.

29. A.

Or

B.

30. A.

Or

B.

(4 x 6 = 24 marks)