K A N N U R U N I V E R S I T Y

(Abstract)

M.Sc Chemistry Course-Scheme and Syllabus-Revised & Implemented with effect from 2010 admission- Orders Issued.

ACADEMIC BRANCH

U.O.No.Acad/C2/8961/2008 Dated, K.U.Campus.P.O, 27-05-2010.

Read: 1. U.O.No.Acad/C2/3168/2001 dated 03-06-2004.

2. Minutes of the meeting of the Board of Studies in Chemistry (PG) held on 23-09-2008 & 28-04-2009.

3. Minutes of the meeting of the Faculty of Science held on 19-06-2009.

4. Item No.I B(iii) of the minutes of the ninth meeting of the Academic Council held on 16-02-2010.

O R D E R

1. The Scheme and Syllabus of M.Sc Chemistry Course were implemented in this University with effect from 2004 admission as per paper read (1) above.

2. The Board of Studies in Chemistry(PG) at its meeting held on 23-09-2008 & 28-04-2009,vide paper read (2) above, has recommended to revise the Scheme & Syllabus of M.Sc Chemistry Course with effect from 2010 admission.

3. The meeting of the Faculty of Science held on 19-06-2009 vide paper read(3) above has passed the recommendation of the Board of Studies on the revision of the Scheme & Syllabus of M.Sc Chemistry Course for the approval of the Academic Council.

4. The Academic Council of the University ,vide paper read(4) above, has resolved to approve the above recommendation of the Board of Studies, as endorsed by the Faculty concerned, with effect from 2010 admission.

5. The Vice Chancellor, after considering the matter in detail, has accorded sanction ***to implement the revised Scheme & Syllabus of M.Sc Chemistry Course, as approved by the Academic Council, with effect from 2010 admission.***

6. The U.O read above, stands modified to this extent.

7. The regulations for Postgraduate Programme under Semester Pattern implemented with effect from 2001 admission is applicable for this Course also.

8. Orders are issued accordingly.

9. The Revised Scheme & Syllabus of M.Sc Chemistry Course effective from 2010 admission is appended.

Sd/-
REGISTRAR

To

The Principals of Colleges offering M.Sc Chemistry Course.

Copy to:

1. The Examination Branch (through PA to CE).
2. The Chairman, BOS in Chemistry (PG).
3. PS to VC/PA to PVC/PA to Registrar.
4. DR/AR-I (Academic)
5. The Computer Programmer (to publish in the Website)
6. SF/DF/FC.

Forwarded/By Order

SECTION OFFICER

K A N N U R U N I V E R S I T Y

COURSE STRUCTURE

&

SYLLABUS

FOR

POSTGRADUATE PROGRAMME

IN

C H E M I S T R Y

w.e.f 2010 ADMISSION

The syllabi of M.Sc. programmes in chemistry offered in the affiliated colleges of the university under semester system has been revised in the light of the decisions of the Board of studies meetings in chemistry (PG). The revised syllabi are to be effective from 2010 admission onwards. There are two independent PG programmes in chemistry, namely M.Sc. Chemistry and M.Sc. Material chemistry. All these M.Sc. programmes are equivalent in all respect for employment and higher studies. Each of these two PG programmes shall extend over a period of two academic years comprising of four semesters, each of 450 hours in 18 weeks duration.

Candidates with Bachelors 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 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. The course consists of four theory papers and three practical papers (to be continued in semester II) in the 1st semester, four theory papers, three practical papers in the IInd semester, four theory papers and three practical papers (to be continued in semester IV) in the IIIrd semester and two elective papers (one compulsory and other optional) three practical papers, a project, a tour report and viva voce in the IVth semester. Each theory 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. 20% of marks shall be allocated for internal assessment of theory and practical papers each. The syllabus and scheme of examination is given below.

SYLLABUS AND SCHEME OF EXAMINATIONS

SEMESTER I

Name of Papers	Hours/ Week	Duration of Exam	Marks for ESA	Marks for CA	Total Marks
(A) THEORY PAPERS					
Paper I – Theoretical Chemistry – I	4	3	60	15	75
Paper II – Inorganic Chemistry – I	4	3	60	15	75
Paper III – Organic Chemistry – I	4	3	60	15	75
Paper IV – Physical Chemistry – I	4	3	60	15	75
(B) PRACTICAL PAPERS					
(TO BE CONTINUED IN SEMESTER – II)					
Paper I - Inorganic Practical – I	3				
Paper II – Organic Practical – I	3				
Paper III – Physical Practical – I	3				
TOTAL MARKS FOR SEMESTER – I				**300**	

SEMESTER II

Name of Papers	Hours/ Week	Duration of Exam	Marks for ESA	Marks for CA	Total Marks
(A) THEORY PAPERS					
Paper V – Theoretical Chemistry – II	4	3	60	15	75
Paper VI – Inorganic Chemistry – II	4	3	60	15	75
Paper VII – Organic Chemistry – II	4	3	60	15	75
Paper VIII – Physical Chemistry – II	4	3	60	15	75

Name of Papers	Hours/ Week	Duration of Exam	Marks for ESA	Marks for CA	Total Marks
(B) PRACTICAL PAPERS					
Paper I – Inorganic Practical – I	3	6	40	10	50
Paper II – Organic Practical – I	3	6	40	10	50
Paper III - Physical Practical – I	3	6	40	10	50
TOTAL MARKS FOR SEMESTER –I1					**450**

SEMESTER III

Name of Papers	Hours/ Week	Duration of Exam	Marks for ESA	Marks for CA	Total Marks
(A) THEORY PAPERS					
Paper IX- Inter Disciplinary Topics and Instrumentation Techniques	4	3	60	15	75
Paper X- Inorganic Chemistry- III	4	3	60	15	75
Paper XI – Organic Chemistry –III	4	3	60	15	75
Paper XII – Physical Chemistry – III	4	3	60	15	75

(B) PRACTICAL PAPERS

(TO BE CONTINUED IN SEMESTER – IV)

Name of Papers	Hours /Week
Paper IV – Inorganic chemistry Practical - II	3
Paper V – Organic chemistry Practical– II	3
Paper VI - Physical chemistry practical– II	3

TOTAL MARKS FOR SEMESTER – III **300**

SEMESTER IV

Name of Papers	Hours /Week	Duration of Exam	Marks for ESA	Marks for CA	Total Marks
(A) THEORY PAPERS (ELECTIVE PAPERS PAPER XIII & XIV)					
Paper XIII –Elective Paper – 1 (Compulsory – Environmental Chemistry)	6	3	75	25	100
Paper XIV – Elective Paper – II*	6	3	75	25	100

Name of Papers	Hours/ Week	Duration of Exam	Marks for ESA	Marks for CA	Total Marks
(B) PRACTICAL PAPERS					
Paper IV – Inorganic Practicals – II	3	6	40	10	50
Paper V –Organic Practicals – II	3	6	40	10	50
Paper VI – Physical Practicals – II	3	6	40	10	50
C) Project Work	4		40	10	50
D) COMPREHENSIVE VIVA – VOCE			40		40
E) STUDY TOUR			10		10

TOTAL MARKS FOR SEMESTER –IV **450**

TOTAL MARKS FOR SEMESTER – 1 to IV **1500**

* One among the following can be chosen as elective paper

1 Organic Polymer and Composite

2. Electro Chemistry and Industrial Catalysis

3. Ceramic and Composite

4. Computational Chemistry

Project work

a) During semester – IV, each student shall carry out a project work in one of the broad areas of Theoretical / Organic / Physical Chemistry / Environmental science for a period of about 10 – 12 weeks under the supervision of a teacher of the Department. The project can be carried out in a research institute / industry of national repute with co guidance from experts there, or in both.

b) The candidate shall submit three copies of the dissertation based on the results of the project work at the end of IVth semester. One external examiner and one internal examiner who is the respective supervising teacher of the department shall value the dissertation. The pass minimum of the project is 50% of the total marks assigned to the project work. Those who obtain less than 50% marks for the project shall resubmit the dissertation in a supplementary appearance after incorporating the modification suggested by the examiners.

c) Viva-voice examination on the project work and elective paper shall be conducted on a separate day by the same team of examiners who valued the dissertation.

d) The student will visit research institute of National repute and submit the report at the end of the fourth semester practical examination.

Internal Assessment:

a) The internal assessment marks shall be awarded based on the performance of the students in the following components. A) Test papers, Seminars, Viva-voce and attendance in respect of each theory paper, and b) Lab skill, model examination, and attendance in respect of each practical paper. The assessment shall be done by a committee of teachers of the Department belonging to the broad area of the concerned paper. The answer paper shall be returned to the students after assessment.

b) The marks scored in each test paper shall be taken after normalization as the internal marks for this component. For seminar/viva the internal mark shall be the average of the marks awarded by the individual teachers in the assessment committee. The internal assessment marks awarded to the students in each paper in a semester shall be notified on the notice board at least one week before the commencement of external examination.

c) A Grievance Redress Committee shall be constituted as and when required to look into the complaints, if any, lodged by the students regarding the marks awarded to them in the internal assessment in each semester.The committee shall consist of the Head of the Department as Chairman, the Departmental Council Secretary or Teacher nominated by the Departmental

Council and the Teacher(s) handling the subject in question. The decision of the Redressal Committee shall be final.

Conduct of External Examination

a)External examination in each semester shall be conducted after five months from the commencement of classes. The Board of Examiners shall consist of one External Examiner and one Internal Examiner from the Department in each of the broad areas of Theoretical/ Inorganic/ Organic/ Physical Chemistry/ Environmental. In the IVth semester all the teachers supervising the project shall be in the Board as Internal Examiners.

b)The Board of Examiners will value the theory papers, conduct practical and viva-voce examination and evaluate the project work. The answer scripts of each paper (theory as well as practical) of external assessment shall be valued by two examiners (one external and one internal) and the average mark is awarded. If the marks awarded by the two examiners differ by more 15% 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 one external examiner and the respective supervising teacher of the Department.The practical examination, viva-voce and project evaluation will be conducted by two examiners among them one will be from the respective institute.

The viva-voce examination will be based on the theory papers/practical papers/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 force at that time.

Instruction to Question Paper Setters

The syllabus of each theory paper has five units. While setting the question papers, equal weight age is to be given to each of units for choosing the questions. Each question paper is of 3 hours duration and has three section, namely Section A, Section B and Section C constituting a total of 60 marks for general papers and 75 marks for elective papers as detailed below.

GENERAL PAPERS		**MARKS**
Section A; 10 out of 12 questions	10x11/2	15
There should be at least two questions from each unit		
Section B; 5 out of 8 questions	5x3	15
There should be at least one question from each unit		
Section C; 5 out of 10 questions	5x6	30

Choice should be limited to the unit. From each unit, out of two questions one question has to be answered.

TOTAL 60

ELECTIVE PAPERS		**MARKS**
Section A; 10 out of 12 questions	10x2	20
There should be at least two questions from each unit		
Section B; 5 out of 8 questions	5x4	20
There should be at least one question from each unit		
Section C; 5 out of 10 questions	5x7	35
Choice should be limited to the unit. From each unit, Out of two questions one question has to be answered.		
	TOTAL	**75**

Allocation of marks for different components of continuous assessment shall be in the following proportions

THEORY

	General		***Elective***	
a)	Attendance	2	Attendance	4
	Attendance less than 75%-0 mark 76-90%-1 mark, More than 90%-2 Marks		Attendance less than 75%-0 mark 76-85%-2 marks, 86-90%-3 marks More than 90%- 4marks	
b)	Seminar	3	Seminar	5
c)	Tests	6	Tests	10
d)	Viva-voce	4	Viva-voce	6
	TOTAL	**15**	**TOTAL**	**25**

PRACTICALS

a)	Attendance (Attendance less than 75%-0 mark, 76-90% - 1mark, more than 90% - 2 marks)	2
b)	Lab skill and presentation of data	3
c)	Model examination	5
	TOTAL	**10**

PROJECT

Presentation in a seminar before the staff members	5
Defense on the project	5
TOTAL	**10**

A student cannot omit any of the components mentioned under continuous assessment.

Sd/-
Dr. Zeinul Hukuman.N.H
Chairman,BOS Chemistry (PG)

SEMESTER-I

PAPER - 1 - THEORETICAL CHEMISTRY I

TOTAL: 70 HOURS

UNIT-1 **14 HOURS**

Quantum mechanics-I:

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 Schrödinger 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-Hermition 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 **14 HOURS**

Quantum mechanics-II:

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 harmonics- 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 **14 HOURS**

Quantum mechanics-III:

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 perturbation method- 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 orbitals -anti symmetric principles- Paul's exclusion principle- Slater determinantal wave functions- 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 **14 HOURS**

Chemical bonding:

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.

UNIT-V **14 HOURS**

Theory of directed valency

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 - H M O theory - application to simple systems (ethylene, allyl systems, butadiene, cyclic conjugated systems and aromaticity (benzene)- bond order, charge density and free valence calculations - Brief discussion of bonding in metals

REFERENCE

I N Levine, ***Quantum Chemistry 5th Ed***. Prentice Hall India

R. Anantharama, ***Fundamentals of Quantum Chemistry***, McMillan India

A. K. Chandra, ***Introductory Quantum Chemistry- 4th Ed***. Tata McGraw Hill

D. A. McQurie ***Quantum Chemistry***, University Science Books

L. Pauling and W. B. Wilson, ***Introduction to Quantum Mechanics***, McGraw Hill

R. K. Prasad, ***Quantum Chemistry 4th Ed***. , New Age International

P. W. Atkins, ***Molecular Quantum Mechanics***, Oxford University Press

M. S. Day and J. Selbin, ***Theoretical Inorganic Chemistry***, East West Books

Tamas Veszpremi and Miklos Feher, ***"Quantum Chemistry- Fundamentals to Applications"***- Springer.

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

PAPER II INORGANIC CHEMISTY – I

TOTAL: 70 HOURS

UNIT-I **14 HOURS**

Theoretical basis of analysis:

Preparation of samples for analysis- sampling statistics-sampling and physical state. Nature of errors- Statistical treatment of errors- Standard deviation for sample and population data- Reliability of results- Confidence level Comparison of results- the 't' and F test- Significant figures- Rejection of data. Precipitation phenomena- Precipitation from homogenous solution- Organic precipitants in inorganic analysis- Extraction of metal ions- nature of extractants- distribution law- partition coefficients- types of extractions and applications. Chelometric titrations- titration curves with EDTA- feasibility of EDTA titration- indicators for chelometric titrations- Selective masking and demasking techniques- Industrial applications of masking.

UNIT-II **14 HOURS**

Acids and bases:

General properties and characteristics of solvents- Self ionization and leveling effect- Effect of substituents on strength of acids and bases- Hard and Soft acids and bases- Classification of Lewis acid as hard and soft bases- Bonding in Hard-Hard and Soft-Soft combinations- HSAB principle and its applications.

Non aqueous solvents:

Reactions in non aqueous solvents- Solute-Solvent interactions- Reactions in liquid ammonia- Solutions of metals in liquid ammonia- Reactions in anhydrous sulphuric acid, liquid sulphur dioxide, liquid HF and liquid dinitrogen tetroxide.

UNIT-III **14 HOURS**

Nuclear and radiation chemistry:

Nuclear structure-mass and charge- Nuclear moments- Binding energy- Semi empirical mass equation- Stability rules- Magic numbers- Nuclear models- Shell, Liquid drop, Fermi gas, Collective and optical models- Equation of radio active decay and growth- half life and average life. Radio active equilibrium- Transient and secular equilibrium- Determination of half lives- Nuclear reactions- Energetics of nuclear reaction- Types of nuclear reactions- Spontaneous and reduced fission- Neutron capture cross section and critical size- Principle and working of GM, Proportional, Ionization and Scintillation counters- Applications of radioactivity

UNIT-IV **14 HOURS**

Nuclear Energy in India

Basic Principles of Nuclear Reactors: Fission and Fusion - Sustainable chain reaction - Nuclear materials, Nuclear fuels, Moderators and Poisons - Conversion and Breeding - Types of Reactors: Pressurized Water Reactor (PWR, VVER), Boiling Water Reactor (BWR), CANDU (Pressurized Heavy Water Reactor - PHWR), GCR (Gas Cooled Reactor), RBMK (Graphite Moderated Nuclear Power Reactor), Liquid Metal cooled Fast Breeder Reactor (LMFBR)

Homi Bhabha and India's Nuclear Power Development Programme -The Three Stages: Targets and Achievements - From Tarapore to Koodankulam. Fuels for India's nuclear weapons programme. The justification for import of fuels and Reactors. The India - US Nuclear Accord. Separation of Civil and Military Programmes. The Planning Commission's vision of the Role of Nuclear Energy in India's Power Development Scenario.

UNIT-V **14 HOURS**

Metal clusters:

Metal carbony1 clusters- Anionic and hydrido clusters- LNCC's and HNCC's- Isoelectronic and isolobal relationships- Hetero atom in metal clusters- Electron counting schemes for HNCC's- Capping rule-Halide type clusters-Chevrel phases and

Zintl Ions- Metal clusters as catalysts.

The neutral boron hydrides- structure and bonding- the topological approach to Boron hydride structure- Styx number- Synthesis and reactivity of neutral boron hydrides- Importance of icosahedral frame work of B atoms in boron chemistry- Closo, nido and arachno structures- Wades rule- Carboranes and metallocrarboranes.

REFERENCES:

F.A Cotton, Wilkinson, C A Murillo and M Bochmann, ***"Advanced Inorganic Chemistry 6th Edition"***, John Wiley and Sons, Inc.

Bodie Douglas, Darl H Mc Daniel and John J Alexander***, " Concepts and models of Inorganic Chemistry"***, John Wiley and Sons, Inc.3rd edition

G N Jeffery, J Basette, J Mendham and R C Denny, ***"Vogel's Text Book of Quantitative Chemical analysis", (Vth Edn)*** John Wiley and Sons, Inc.

H Sisler, ***"Chemistry of Non-acqueous solvents"*** Reinhold.

J E Huhee, ***"Inorganic Chemistry-Principles of structure and reactivity",*** Pearson Education India

G Friedlander and J W Kennedy ***" Introduction to Radiochemistry",*** John Wiley and Sons, Inc.

S Glasston***, "Source book on Atomic energy***", Van Nonstrand.

H.J Arnikar – ***"Essentials of Nuclear Chemistry",*** New Age International, New Delhi.4th Edition 1995

J.D Lee- ***"Concise Inorganic Chemistry " (IVth Edn.)*** Oxford University Press.

S.K Agarwal and Keemti Lal ***"Advanced Inorganic Chemistry"*** Pragati Prakashan 9th Edition 2009

PAPER III - ORGANIC CHEMISTRY-I

TOTAL: 70 HOURS

UNIT-I **14 HOURS**

Aromaticity and Molecular rearrangements –

Aromaticity-principles of aromaticity, antiaromaticity, Homo, hetero and non benzenoid aromatic systems- Aromaticity of annulenes, mesoionic compounds, metallocenes, cyclic carbocations and carbanions-

Molecular rearrangements: Mechanism, with evidence of Wagner- Meerwein, Pinacol, Demjanov, Hofman, Curtius, Schmidt, Lossen, Beckmann, Wolff, Fries, Fischer Hepp, Hoffmann-Martius, Von Richeter, Orton, Bamberger, Smiles, Dienone-phenol, Benzilic acid, Benzidine, Favorskii, stevens, wittig Sommelet-Hauser, Baeyer-villiger, and borane rearrangements- Darkin reaction.

UNIT-II **14 HOURS**

Structure, reactivity and intermediates:

Electronic effects- inductive, electromeric,and mesomeric effects- Hyperconjugation- steric effects- 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, formation and reactions- Carbon fradical: structure, formation and stability, Radical reactions, auto oxidation and radical chain reactions- structure, stability and formation of carbocations and carbanions-

UNIT-III **14 HOURS**

Stereochemistry of organic compounds:

Molecular chirality and stereochemical nomenclature-molecules with chiral axes and planes- molecular shape, topology and optical activity-Atropisomerism and its designation- racemisation- resolution- prostereoisomerism- stereotopicity and enantiomeric excess- Non carbon chiral centers- Introduction to ORD, CD and their application in assigning configuration and conformation- octant and axial haloketone rules- conformational analysis of cycloalkanes, decalins and their substituted derivatives.

UNIT-IV **14 HOURS**

Substitution and elimination reactions:

Neucleophilic substitution at sp^3 carbon- its mechanism and stereochemical aspects- effect of solvent, leaving group and substrate structure- Neighboring group participation- Non classical carbocations- Aromatic nucleophilic substitutions – 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.

UNIT-V **14 HOURS**

C-C and C=C bond forming reactions- Mannich, Reimer-Tiemann Simon-Smith, Vilsmeier, Haack, Roformatsky and Ulmann reactions, Stork Enamine Reactions, Shapiro, Witting-Horner, Peterson,

Heck, Still and Mc Murray reactions- Ring Formations by Dieckmann, Thorpe and Acyloin condensations- Robinson ring annuolation- synthesis of small rings- simon-smith reactions reduction and oxidation in synthesis- catalytic hydrogenation- alkali metal reduction- Wolf Kishner reduction- Huang Million Modification- Clemmenson Reduction- Boranes- LAH, Sodium Borohydride as reductants- Dehydrogenation- oppenaur oxidation- HIO_4, OSO_4 and ClC_6H_4COOH and their applications

REFERENCES

D Nasipuri, ***"Stereochemistry of Organic Compounds"***, Wiley Eastern.

P Y Bruice, ***"Organic Chemistry"***, Prentice Hall.

P Sykes, ***"A Guidebook to Mechanisms in Organic Chemistry"***, Longman.

S N Issacs, ***"Physical Organic Chemistry,"*** Longman.

M B Smith, ***"March's Advanced Organic Chemistry,"*** 5th Edn,Wiley (or earlier editions of J March.

F A Carey and R S Sundberg, ***"Advanced Organic Chemistry 4th Edn.,"*** Part A and B, Kluwer,

M A Fox and J K Whitesell, ***"Organic Chemistry,"*** 2nd Edn, Jones and Barlett.

C J Moody and W H Whitham, ***"Reactive Intermediates,"*** Oxford University Press.

I L Finar, ***"Organic Chemistry," Vol 2,*** Longman.

PAPER IV PHYSICAL CHEMISTRY-I

TOTAL: 70 HOURS

UNIT-I **14 HOURS**

Thermodynamics:

A brief resume of laws of thermodynamics. Entropy as a measure of unavailable energy-concept of fugacity and free energy-Variation of free energy with T and P-Maxwell's relations- Nernst heat theorem and its applications. Third law of thermodynamics-determination of absolute entropies. Unattainability of absolute zero-Residual entropy

Applications of thermodynamics: Entropy and free energy of mixing-.Partial molar quantities-

Chemical potentials- General methods for the determination of partial molar properties- Deviation from Raoults law-Gibbs Duhem and Gibbs Duhem Margules equation-Excess thermodynamic functions

Thermodynamics of irreversible process: Simple examples of irreversible process. Entropy production-heat flow- matter flow- chemical reaction. The phenomenological relations- Onsager reciprocal relation. Thermo osmosis and thermo molecular pressure difference- Thermo electricity.

UNIT-II **14 HOURS**

Phase equilibria:

Physical equilibria involving phase transition- criteria for equilibrium between phase-Three component system- graphical representations- solid liquid equilibria- Ternerary 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 III **14 HOURS**

Electro chemistry:

conductance measurements- Technique at a high frequency and high voltage- Results of conductance measurements- ionic motilities- Influence of pressure and temperature on ion conductance- Walden's equation- Abnormal ion conductance- Derivation of Debye-Huckel-Onsager equation-validity of Debye-Huckel-Onsanger equation for acqueous and nonaqueous solution- Deviation from Onsager equation- Conductance ration 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 coefficeient- Ion association- dissociation constant- Tripple ion and conductance minima- Equilibria in electrolytes- Association constant- solubility product principle- solubility in presence of common ion-Activity coefficient and solubility measurement.

UNIT IV **14 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 multi layer capacity Electric capillary- Lippmann potential-

Membrane potential- Polarization- electrolytic polarization. Dissolution and decomposition potential- concentration polarization. Over voltage- Hydrogen and Oxygen over voltages- theories of over voltage- Butler volume equation for simple electron transfer reaction- Transfer coefficient- Exchange current density Rate constants- Tafel equation and its significance- Principle and application of polarography and amperometry.

UNIT V **14 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

Rastogi and Misra-***"An Introduction to chemical thermodynamics-6th edition***"– Vikas publishing.

S. Glasstone- "***Thermodynamics for chemists***" – Affiliated East West publication.

Lewis and Randall- "***Thermodynamics***"- Mc Graw Hill.

Daniels and Alberty- "***Physical Chemistry***"- John Wiley.

S. Glasstone- "***Theoretical electrochemistry***"- East West Books

L.I. Anthropov- "***Theoretical electrochemistry***"- Mir publishers.

Bockris and Reddy- "***Modern electrochemistry***"- Springer 2nd Edition volumes 1, 2A and 2B

G.W. Castellon ***"Physical chemistry***"- Narosa

I. Pregogine- ***"Introduction of Irreversible to thermodynamics process"-*** Interscience.

G.M.Barrow- ***Physical chemistry***- TataMcGraw Hill.

Dutta K.Robin "***Physical Chemistry***"Ane Books

Winston Revie and Herbert Uhlig ***Corrosion and corrosion control***: (Wiley)

SEMESTER-II

PAPER-V THEORETICAL CHEMISTRY-II

TOTAL: 70 HOURS

UNIT-1 **14 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-.

UNIT-II **14 HOURS**

Theory of molecular symmetry

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- 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).

UNIT-III **14 HOURS**

Applications of group theory

Applications to molecular vibrations- symmetry aspects of molecular vibrations-vibrations of polyatomic molecules- selection rules for vibrational absorption- complementary character of I R and Raman spectra- determination of the number of active I R and Raman lines. Applications to chemical bonding- construction of bybrid orbitals-BF_3, CH_4, $PC1_5$ as examples- transformation properties of atomic orbitals. Application to MO theory of H_2O, NH_3 and octahedral complexes.

UNIT-IV **14 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 vibrationos, fundamental, overtones and hot bands- Degrees of freedom of poly atomic molecules and nature of molecular vibrations(eg CO_2 and H_2O), vibration-rotation spectra of diato,mic 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, vibratiobnal-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-V **14 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

F A Cotton, ***"Chemical Applications of Group Theory"*** Wiley Eastern.

L H Hall ***"Group Theory and Symmetry in Chemistry"***, McGraw Hill.

V Ramakrishnan and M S Gopinathan, ***"Group Theory in Chemistry"*** Vishal Publications, 1992.

Banwell and Mc Cash "***Fundamentals of Molecular Spectroscopy"***, Tata McGraw Hill

G Aruldas ***"Molecular Structure and Spectroscopy***", Prentice Hall,

Manas Chanda ***"Atomic Structure and Chemical Bonding including Molecular Spectroscopy, 4th Edn,***" Tata McGraw Hill

Barrow ***"Molecular Spectroscopy,"*** McGraw Hill.

P W Atkins "***Physical Chemistry***," ELBS

S Swarnalakshmi, T Saroja and R M Ezhilarasi "***A Simple Approach to Group Theory in Chemistry***"- Universities Press

Thomas Engel "***Quantum Chemistry and Spectroscopy***"- Pearson.

Quinn ***"Computational Quantum Chemistry-II: The Group Theory Calculator***"- -AneBooks

H.Kaur **"Spectroscopy"** 3rd Edition Pragati Prakasan Meerut

TOTAL: 70 HOURS

UNIT-1 **14 HOURS**

Chemistry of transition elements and Co ordination chemistry:

Coordination numbers 2 to 12 and geometry- limitations of VB theory- 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- hydration and ligation- MOT in coordination compounds- MO energy level diagrams for octahedral, tetrahedral and square planar configuration with and without π bonding- MOT, a group theoretical approach- Angular overlap model of bonding in complexes- Effect of π bond in stability- Nephelauxetic series- critical comparison of the three theories as applied to metal complexes.

UNIT-II **14 HOURS**

Spectral and magnetic properties of complexes:

Term symbol for d^n ions, spectroscopic ground states- selection rules for d-d transitions- nature of spectral bands- band shapes, band intensities, band widths, spin orbit coupling- vibrational structures- Orgel diagrams of transition metal complexes (d^1 to d^9 configuration) – Tanabe Sugano diagrams Interpretation of spectra of spin paired and spin free octahedral, distorted octahedral, tetrahedral and square planar complexes- charge transfer transition- Origin, types and characteristics.

Types of magnetic behaviors- magnetic susceptibility measurements- Gouy method diamagnetic corrections- spin only value- orbital contribution- spin orbit coupling- ferro and antiferro magnetic coupling- spin cross over systems- Application of magnetic measurements to structure determinations of transition metal complexes.

UNIT-III **14 HOURS**

Instrumental methods of studying coordination complexes:

Optical activity in coordination complexes- ORD and CD- cotton effect- applications. Infra red spectroscopy: Changes in band positions- band intensities and band splitting for assigning proper geometry for complexes- Illustrations with proper examples. Nuclear Magnetic Resonance- Nuclear Quadrupole Resonance- Mossbauer and Electron Spin Resonance Spectroscopy for structural studies of complexes- Importance of molar conductance studies in coordination Chemistry.

UNIT IV **14HOURS**

Reaction of metal complexes:

Metal ligand equilibria in solutions- Step wise and overall formation constants (stability constants)- chelate effect- Irwing- William order of stability. Factors affecting the stability of metal complexes- Determination of binary formation constants by P^H metry and spectrophotometry- Energy profile of a reaction- inert and labile complexes- kinetics of octahedral substitution, acid hydrolysis, base hydrolysis- anation reactions- reactions without M-L bond cleavage- substitution reaction in

square planar complexes- trans effect- mechanism of substitution- redox reaction- inner sphere and outer sphere reactions- complimentary and non complimentary reactions.

UNIT V **14 HOURS**

Organo metallic chemistry

Compounds with metal – carbon single bonds- alkyls and aryls of Li, Be, Mg, Al, Sn and Pb Preparation, reactions and bonding- Applications (catalytic) Transition metal alkyls and aryls – Routes of synthesis- stability and decomposition pathways- Organo copper in organic synthesis – Transition metal to carbon multiple bonded compounds alkylidines,alkylidynes-low valent carbines and carbenes.Synthesis-nature of bond, structural characteristics and reactivity- (electrophilic and nucleophilic reactions on the ligands)

REFERENCES

S. F A Kettle, ***"Coordination Chemistry."*** Thomas Nelson and Sons

J C Bailar, ***"Chemistry of coordination compounds."*** Reinhold.

F Basolo R Johnson, ***"Coordination Chemistry,"*** Benjamin Inc.

D Banergea, ***"Coordination Chemistry,"*** Tata McGraw Hill.

D N Sathyanarayana, ***"Electronic Absorption Spectroscopy and related Techniques,"*** Universities Press.

R Gopalan and V N Ramalingam, ***"Concise Coordination Chemistry,"*** Vikas publishing Hourse Pvt Ltd.

M C Day and J Selbin, ***"Theoretical Inorganic Chemistry,"*** Affiliated East West Press.

J E Huhee, ***"Inorganic Chemistry-Principles of structure and reactivity"***, Pearson Education India

R L Dutta and A Syamal, ***"Elements of magneto Chemistry"*** S Chand & Company Ltd.

Glen E.Rodgers **"Inorganic and Solid state Chemistry"** Ceengage Learning

Indrajit Kumar **"Organometallic compounds"** Pragati prakasan Meerut

PAPER-VII ORGANIC CHEMISTRY-II

TOTAL: 70 HOURS

UNIT-1 **14 HOURS**

Pericyclic reactions:

Classification of pericyclic reactions-Woodward Hoffmans rule, mechanism and stereo course of electrocylic, cycloaddition and sigmatropic reactions.Analysis of electrocyclic and cycloaddition reactions by FO and Correlation Diagram methods. Analysis of sigmatropic reactions by FO method. [3,3] migrations- Claisen and Cope rearrangements. Huckel Mobius analylsis of electrocyclic , cycloaddition and sigmatropic reactions- Stereoaspects of Diels Alder reaction- Retro Diels-Alder reactions - Fluxional molecules-, Ene, Chelotropic and cis elimination reactions- Synthetic applications

UNIT-II **14 HOURS**

Organic Photochemistry:

Photochemical processes- Energy transfer- sensitization and quenching- singlet and triplet states and their reactivity- photoreactions of carbonyl compounds, enes, dienes and arenes- Norrish reaction of acyclic ketones- Patterno-Buchi Burton, photo-Fries and Di-π methane rearrangement reaction- Photoreactions of vitamin D- photochemistry of vision and photosynthesis- singlet oxygen generation and reactions- Application of photoreaction in laboratory and industrial syntheses.

UNIT-III **14 HOURS**

Chemistry of natural products:

Structure and synthesis of alpha pinene, Camphor, Cadenine and Caryophyllene- Hofmann, Emde and von Braun degradation in alkaloid chemistry- structure elucidation of papaverine, Quinine and Morphine- Synthesis of Quinine and papaverine- structure and synthesis of beta-carotene, Flavone, Isoflavone, Cyanin and Quercetin- Biosynthesis of terpenes and alkaloids- classification and structure of lipids and their biofunctions- Nomenclature, structure (not elucidation) and biosynthesis of Prostaglandins PGE_2 and $PGF_{1\alpha}$

UNIT-IV **14 HOURS**

Chemistry of Biomolecules: Nomenclature, reactivity and stereochemistry of steroidal systems-stereochemistry and structure elucidation of cholesterol . structure and synthesis of Testosterone, Andestrone, Estrone and Progesteron- Steroid biosynthesis- structure and synthesis of vitamin A, C, B_1 and Biotin- Structure of Penicillins- Synthesis of Paracetamol, Phenobarbital, diazepam, sulphamethoxazole, benzylpenicillin and chloramphenicol.

UNIT-V **14 HOURS**

Chemistry of Biopolymers: FMOC, BOC, Z, trityl, phthalimide and benzyl protecting groups-Peptide bond formation by carbodimide and active ester methods in SPPS- Helical and sheet conformations of polylpeptides- Structure organization of proteins- Chemistry of nucleic acid bases A, G, C, T and U and their synthesis- Synthesis of adenosine and ATP- Structure of DNA- Automated oligonucleotide

synthesis by phosphoramidite method- Reagents and protecting groups- Sequencing of polynucleotides and polyperptides- Structure of starch cellulose, Glycogen and Chitin.

REFERENCE

L M Harwood, "***Polar Rearrangements,***" Oxford University.

J March, "Advanced ***organic Chemistry***" Wiley India

S N Issacs, "***Physical Organic Chemistry***." Longman.

P Y Bruice, "Organic ***Chemistry,***" Pearson Education

H Aroara, ***"Organic Photochemistry and Pericyclic Reactions***" Anmol Publications

C H Dupuoy and O L Chapman, "***Molecular Reactions and Photochemistry,"*** Prentice Hall.

J M Coxon and B Holtom. "***Organic Photochemistry***, Cambridge University press.

S H Pine, ***" Organic Chemistry***," Tata McGraw Hill.

I L Finar, "***Organic Chemistry***," Vol 2, Pearson Education

J Kagan, "***Organic Photochemistry***," Academic Press.

R J Simmonds, "***Chemistry of Biomolecules***," Royal Society of Chemistry.

J Mann and others, "***Natural Products- Their Chemistry and Biological Significance***," Longman.

Alka L.gupta, "***Medicinal Chemistry***," Pragati Prakasan Meerut

N.R.Krishnaswamy '***Chemistry of Natural Products– A Unified Approach'***. University Press

S.K Ghosh **"Advanced General Organic Chemistry"**Part1and11 New Central BookAgency

AhluwaliaV.K.,MaduChopra "***Medicinal Chemistry***," Ane books

PAPER-VIII PHYSICAL CHEMISTRY-II

TOTAL: 70 HOURS

UNIT-1 **14 HOURS**

Statistical Thermodynamics:

Basic principles: permutation- probability concept Thermodynamic probability- Microstates and microstates- Derivation of Boltzmann distribution law- Partition function- physical significance- Different ensembles- canonical partition function- Distinguishable and Indistinguishable molecules- Partition function and thermodynamic function- Separation of partition function- Translation partition function. Rotational, vibrational and electronic partition function. The calculations of thermodynamic functions and equilibrium constants- Equation of state- Saleur Tetrode equation- Statistical formulation of third law of thermodynamics- Basis idea of phase-space. Heat capacity of gases-classical and quantum theories- Heat capacity of Hydrogen- ortho and paraHydrogen.

The atomic crystals: Einstein's theory of atomic crystal-Debye's modification of Einstein's model.

UNIT II **14 HOURS**

Imperfect gases:

The virial expression and virial coefficient- relation between virial coefficient and the cluster integrals. 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.

UNIT III **14 HOURS**

Liquid state:

X-ray diffraction study of simple liquids and their structure- Configurational partition function for liquids- Theories of liquid state: oscillator, free volume and VanderWaals theories- Lennard-Jones theory of melting-communal entropy- specific heat of liquids.

Liquid crystals: Mesomorphic state- types, examples and application- Theories of liquid crystals- photoconductivity of liquid crystals.

UNIT-IV **14 HOURS**

Solid state:

Classification of solids into conductor, semiconductor and insulators. Imperfection in solids- point, line and plane defect. Electrons and holds. Nonstoichiometry. Imperfection and physical properties of solids (brief survey).

1. Electrical properties- electrical conductivity- Hall effect- dielectric properties piezoelectricity, Ferro electricity and conductivity.
2. Optical properties- Photo conductivity-luminescence-color center- lasers- refraction-birefringence.

3. Magnetic properties- diamagnetism- paramagnetism- Ferro, antiferro and ferrimagnetisms- Calculation of magnetic moments.

4. Mechanical and thermal properties.

UNIT –V **14 HOURS**

Photochemistry:

Laws of photochemistry- quantum yield- Chemiluminescence- thermo luminescence photosensitization- flash photolysis- pulse radiolysis. Hydrated electron H_2-$C1_2$ and H_2-Br_2 reactions. Photo stationary states. Demerisation of anthracene- Ozone layer in atmosphere Chemistry of photosynthesis and photography- Principle of utilization of solar energy solar cells and their working- Jablonski diagram- Florescence-quantum efficiency of florescence.

Quenching of fluorescence- stern-Volmer equation-Delayed fluorescence-E0type and p-type phosphorescence.

REFERENCES

M.C. Gupta- "***Elements of Statistical Thermodynamics***- New age international.
L.K Nash- "***Elements of statistical Thermodynamics***- Addison Wesley publishing Co.
Kistin andSorfuran- "***A course on Statistical Thermodynamic***"- Academic 1971.
D.A. Mc Quarrie- "***Statistical Thermodynamic***"- Harper and Row 1973.
JAK Tareen and TRN Kutty**"A Basic course in Crystallography"** Universities Press
I.V. Azaroof- "***Introduction to Solids***"- Mc Craw Hill.
Thomas Engel Philip Reid- "***Physical Chemistry***"- Pearson
Alka.L.Gupta- "***Photochemistry***"- Pragati prakashan Meerut.
Dupuy and Chapman- ***"Molecular Reaction and Photochemistry"***- Prentice Hall.

PAPER I

INORGANIC PRACTICALS – I

TIME: 125 HOURS

I. Separation and identification of four metal ions of which two are rare / less familiar such as TI, W, V, Se, Te, Ti, Ce, Th, Zr, U, Mo and Li. (interfering acid radicals not present). Confirmation by the spot test.

II. Volumetric estimation

a) EDTA-Al, Ba, Ca, Cu, Fe, Ni, Co, Hardness of water.

b) Cerimetry- Fe (II), Nitrate.

c) Potassium iodate- Iodide, Sn (II)

III. Colorimetric determinations of Cr, Fe, Ni and Mn.

REFERENCES

G h Jeffrey, J Bassette, J Mendham and R C Denny, "Vogel's Text Book of Quantitative Inorganic Analysis", Longman, 1999.

G.S. Vehla, "Vogel's Quantitative Inorganic Analysis", (7^{th} Edn), Longman (2001).

PAPER II

ORGANIC PRACTICALS-I

TIME : 125 HOURS

1. General methods of separation and purification of organic compounds with special reference to :

a) Solvent extraction

b) Fractional crystallization

c) Steam distillation and distillation under reduced pressure.

d) Sublimation

2. Analysis of organic binary mixtures: Separation and identification of organic binary mixtures containing one component with at least two substituents. (A student is expected to analyze at least 12 different binary mixtures). Identification of the compounds by the determining the physical constants of the components of the mixture and the melting points of the derivatives (by referring tables)

3. Preparation of organic compounds: Single stage preparations by reaction involving nitration, halogenation, oxidation, reduction, alkylation, acylation, consideration and rearrangement. (A student is expected to prepare at least 15 different organic compounds by maing use of the reactions given above).

REFERENCES

A I Vogel "***A Text Book of Practical Organic Chemistry***", , Longman.

A I Vogel "***Elementary Practical Organic Chemistry***", , Longman.

F G Mann and B C Saunders '***Practical Organic Chemistry***", , Longman.

PAPER III

PHYSICAL PRACTICALS – I

TIME: 125 HOURS

(A minimum of 30 experiences to be done covering all units.)

1. Phase rule

(a) Distribution law: Partition of iodine between water and carbon tetrachloride. Equillibrium constant of $I+I_2 \rightleftharpoons I_3$. Concentration of unknown potassium iodide. Partition of ammonia between water and chloroform. Equilibrium constant of $Cu^{2+} + 4NH_3 \text{--} Cu(NH_3)_4^{2+}$. Partition of aniline between 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 liquid systems: Construction of phase diagrams of two component liquid systems. Zeotropic and Azeotropic.

(e) Three component systems: With one pair of partially miscible liquids. Construction of phase diagrams and 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 – Rast method and transition temperature method.

Molecular weight of a solid using a solid solvent by cooling curve method. (solvents – naphthalene, biphenyl, m-dinitrobenzene, p-dichlorobenzene).

Molecular weight determination by study of depression in transition temperature

(Sodium acetate, Sodium thiosulphate and Strontium chloride).

4. **Cryoscopic study** of $2KI + HgI_2 \rightarrow K_2HgI_4$ reaction in water and determination of concentration of KI solution.

5. **Distribution Law**

Distribution coefficient of I_2 between CCI_4 and H_2O.

Study of equilibrium $KI + I_2 \rightarrow KI_3$.

Determination of concentration of KI solution.

6. Refractometry

Determination of molar refractions of pure liquids (water, methanol, ethanol, chloroform, carbon tetrachloride, glycerol).

Determination of composition of mixtures (alcohol-water, glycerol – water, KCl – water).

7. **Viscosity**

Determination of viscosity of pure liquids (water, methanol, ethanol, glycerol, benzene, nitrobenzene, carbon tetrachloride).

Composition of binary liquid mixtures (benzene – nitrobenzene, water – alcohol)

Determination of molecular weight of a polymer (polystyrene in toluene).

8. **Potentiometry**

Electrode potentials of Zn and Ag electrodes in 0.1M and 0.001M solutions at 25^0C and determination of standard potentials.

Mean activity co-efficient of an electrolyte at different molalities by EMF method. Dissociation of strength of the given HCl solution by differential potentiometric titration. Dissociation constant of acetic acid in DMSO, DMS, acetone and dioxin by titrating with NaOH.

Potentiometric titration.

Mixture of chloride and iodide

Mixture of HCl and HAc.

REFERENCES

A. Findlay and J A Kitchener, "***Practical Physical Chemistry***", Longman.

F Daniels and J H Mathews, "***Experimental Physical Chemistry***", Longman.

A M James, "***Practical Physical Chemistry***", J A Churchill.

H H Willard, L L Merritt and J A Dean, "***Instrumental Methods of Analysis***", Affiliated East West Press.

D P Shoemaker and C W Garland, "***Experimental Physical Chemistry***", McGraw Hill.

W.G. Palmer, ***Experimental Physical Chemistry***, Cambridge University Press.

PAPER IX- INTER DISCIPLINARY TOPICS AND INSTRUMENTATION TECHNIQUES

Unit I **14 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 molecules and multiple recognition. - amphiphile organization, supra molecular design strategy & nanotechnology. Supramolecular devices. Supramolecular photochemistry supramolecular electronic, ionic and switching devices.

Unit II **14 Hours**

Computers for Chemists:

Introduction to computers and Computing, Computer languages. Developing of small computer programmes using C language, involving simple formulae in Chemistry, such as Van der Waals equation. Chemical kinetics (determination of Rate constant) Radioactive decay (Half Life and Average Life). Determination of Normality, Molarity and Molality of solutions. Evaluation Electro negativity of atom and Lattice Energy from experimental determination of molecular weight and percentage of element organic compounds using data from experimental representation of molecules in terms of elementary structural features such as bond lengths, bond angles, dihedral angles, etc.

Unit III **14 Hours**

Green Chemistry:

Introduction, the need of green chemistry, principles of green chemistry, planning of green synthesis, tools of green chemistry, Green reactions, Aldol condensation, Cannizaro reaction and Grignard reaction- comparison of the above with classical reactions- Green preparations, Applications phase transfer catalysts, Introduction to Microwave organic synthesis, Applications: environmental, solvents, time and energy benefits

Unit IV **14 Hours**

Nano Science and Technology:

Introduction, nanostructures: tubes, fibers, wires, bricks and building blocks, nanostructure formation: lithography, self-assembly,molecular synthesis,crystal growth and polymerization, measurement of nanostructure: spectroscopy,microscopy and electrochemistry, nanoCAD, Material study: nanocomposites, consumer goods, 'smart materials,' Applications to various fields:optics, telecommunication, electronics, digital technology and environment, Biomedical applications: diagnosation, protic engineering, mapping of genes, drug delivery, biomimetics, quantum dots.

Unit V **14 Hours**

Instrumentation Techniques:

Principles, instrumentation and applications of Thermogravimetry, Differential thermal analysis, Differential Scanning Calorimetry, Dynamic Mechanical Analyzer, Thermo Chemical Analyzer, Direct injection enthalpimetry 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 principle-hyperfine coupling-the 'g' values-isotropic and anisotropic hyperfine coupling constants-zero field splitting and Kramers degeneracy-application to simple inorganic and organic free radicals and to inorganic complexes

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

REFERENCES

Green chemistry, ***V.K.Ahluwalia***, Ane books

P.T. Anastas and J.C.Warner ***Green chemistry***, , Oxford

G.A.Ozin, A.C. Arsenault ***Nano chemistry***, RSC

Diwan, Bharadwaj, ***Nanocomposites***, Pentagon

V.S.Muralidharan A.Subramania, ***Nanoscience and Technology*** Ane Books

B K Sharma, ***Instrumental Methods of Chemical Analysis***, Goel publishing house,2000.

Chatwal Anand, ***Instrumental Methods of Chemical Analysis 7th edition*** Willard 1999.

Skoog, Holler and Nieman, ***Principles of Instrumental Analysis***, Harcourt Brace College Publishers, Philadelphia.

H H Willard, L L Merrit and J J Dean, ***Instrumental Methods of Analysis***, 7th edition, Wadsworth Publishing Company,

G D Christian, Analytical ***Cchemistry***, John Wiley 4th edition,1986

K. V. Raman, ***Computers in Chemistry*** Tata McGraw Hill

Katsuhiko Ariga and Toyoki Kunitake ***Supramolecular Chemistry – Fundamentals and Applications*** Springer

PAPER-X :

INORGANIC CHEMISTRY – III

TOTAL : 70 HOURS

UNIT I **14 HOURS**

Metal Extraction by reduction of oxide ores –

Thermodynamic aspects of extraction. Ellingham diagrams – Chemical and electrolytic reduction-reduction potentials –effect of complexation- Latimer and Frost diagrams – trends in stability of oxidation states, stereo chemistry and ionic sizes of transition metals. Comparison of 3d, 4d and 5d series by taking Ti subgroup as examples.

Lanthanides: Electronic structure, oxidation states – Chemical Properties of +2, +3 and+4 oxidation states Lanthanide and actinide contraction- spectral and magnetic properties. Coordination number and stereochemistry of complexes.

Actnides: Electronic structure- Oxidation states Lanthanide and actinide contraction – spectral and magnetic properties in comparison with those of lanthanide and d-block elements. Trans- actinide elements – IUPAC nomenclature – Periodicity of trans actinide elements.

Beach sands of Kerala – Important components and their separation – Utilization of monazite – illmenite,zircon and sillimanite.

UNIT II **14 HOURS**

Inorganic polymers:

Types of Inorganic polymers – Characteristics of polymers - molecular masses and their distribution – structural features – chain characteristics - solubility consideration – crystalline and mechanical properties.

Polyphosphazenes - Synthetic routes to various types of Polyphosphazenes – important applications of these Polymers – water soluble bioactive Polymers – Organometallic Polyphosphazenes – Polymer bound platinum anti tumour agents.

Polysiloxanes and related Polymers – preparation, structural features and uses – Polysilanes and related Polymers – Chemical modification of Polysilanes – Electrical conductivity and photo conductivity – Polysilanes as photo resists and photo inhibitors.

UNIT III **14 HOURS**

Organometallic chemistry:

Compounds with metal to Carbon single bonds – alkyl and aryls of main group elements – Transition metal to carbon multiple bonds - Metal carbonyls, cyanides and isocyanides – Usefulness of eighteen electrons rule to predict formulae and stability of organometallic compounds.

Transition metal π complexes with alkenes, alkynes, alkynes, allyl, diene, dienyl and trienyl radical – Cyclic π complexes with cyclobutadiene, cyclopentadienyl,arenes, cycloheptatrienyl cyclooctatetraene and cyclooctatetraenyl dianion. Preparation, properties, nature of bonding and structural features –

Fluxionality in π complexes – catalysis by organometallic compounds- hydrogenation, hydroformylation and polymerization reactions.

UNIT IV **14 HOURS**

Bioinorganic Chemistry I

Role of metal ions in the biological system. Essential and nonessential elements – macro minerals and essential trace elements – synergism and antagonism among essential trace elements.

Metal deficiency and diseases related – iron, Zinc and copper deficiency – metal ion toxicity – copper over load and Wilson's disease – iron toxicity – toxicity of arsenic, cadmium, mercury and lead.

Metal complexes in medicine – Chelation therapy – BAL, penicillamine, Polyamino carboxyclic acids and desferrioxamine – gold compounds and rheumatoid arthritis – platinum complexes as anticancer, drugs – metal complexes in radio diagnosis and magnetic resonance imaging.

Metal storage and transport: Iron storage and transport – transferrin, ferritin and siderophores. Other storage and transport systems – ceruloplasmin and serum albumin for copper, metallothioneins and phytochepatins – vanadium storage and transport.

Transport and storage of dioxygen – hemoglobin and myoglobin – structure and functions – structural model for dioxygen binding – co-operativity, Perutz mechanism and Bohr effect – synthetic oxygen carriers. Other natural oxygen binding proteins – hemocyanin and hemerythrin – synthetic model for hemocyanin.

UNIT V **14 HOURS**

Bioinorganic Chemistry II

Electron transfer in biology – structure and functions of electron transfer proteins – Cytochromes and respiratory chain, iron-sulphur proteins rubredoxin and ferridoxins – synthetic models (for Fe_4S_4 cluster only) – blue copper proteins.

Nitrogen fixation: Invitronitrogen fixation through dinitrogen complexes - nitrogen fixing micro organisms – nitrogenases – model compounds.

Photosynthesis: Structure of Chlorophyll – Photo systems I & II – Light reaction – role of manganese enzymes in the cleavage of water. The 'Z –scheme – dark reactions.

Metalloenzymes: Structure and functions of the following enzyme – carbonic anhydrase, carboxy peptidase, alchoholdehydrogenase, catalalse and peroxidase, Cytochrome P-450, super oxide dismutase and xanthin oxidase – B_{12} coenzymes – $B_{12a,}$ B_{12x}, B_{12r} and methyl cabal amine – biomethylation.

REFERENCES

J.E. Huheey, E.A Keiter and RL Keiter: '***Inorganic chemistry Principles of structure and Reactivity***' – Pearson Education

DF Shriver, PW – Atkins – '***Inorganic chemistry***, Oxford university press.

Cotton, Wilkinson, Murillo, Bachmann '***Advanced Inorganic Chemistry'*** Wiley India Pvt.Ltd

B.Douglas, D.MeDaniel and J.Alexander – '***Concepts and models of Inorganic Chemistry IIIrd Edition***. John Wiley & sons, Inc

S.J Lippard and J.M Berg. Principles of ***Bioinorganic chemistry*** University Science Books, California.

David E.Fenton, '***Bio coordination Chemistry***' Oxford University press.

I Bertini, H.B.Grey, S.J.Lippard and J.S Valentine, '***Bioinorganic Chemistry'*** Viva Books Pvt Ltd, New Delhi.

DMP Mingo's, '***Essential Trends in Inorganic Chemistry'*** Oxford University Press.

Indrajeet Kumar ***Organometallic compounds*** Pragati Prakasan,Meerut

PAPER –XI ORGANIC CHEMISTRY-III

Unit I **70 Hours**

Introduction to Spectroscopy Techniques

Electronic transmission in enes. eones and arenes, Woodward Fieser rules – effect of solvent polarity on UV absorption- principles of characteristic group frequency in IR- identification of functional groups and other structural features by IR- Hydrogen bonding and IR bands- sampling techniques- FTIR and its Instrumentation-

Organic Mass Spectroscopy- EI, CA, FAB, electro spray and MALDI ion sources- Magnetic High resolution (Double focusing), TOF and Quadrupole Mass Analysers- Charecteristic fragmentation modes and MS rearrangement – MS-GC, HPLC-MS, TG-MS

Unit II **14 Hours**

NMR spectroscopy and structure elucidation, 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 2DNMR, ^{13}C NMR and ^{13}C Chemical shifts - spectral interpretation and structure identification- spectral interpretation using actual spectra taken from standard texts- solving of structural problems on the basis of numerical and spectrum based data- NMR Spectroscopy of N, F and P –

Unit III **14 Hours**

Reagents and Organic Synthesis: Application of Hydrogenation catalysts- Hindered Boranes- Bulky metal hydrides- NaCN, BH_3, DIBAL, Li trialkyle borohydrides, tri-n-butyl tin hydride, diimide, Lindlar catalysts and Rosenmund redudctions,McFedeyan-stevens reaction- Oxidation using SeO_2, lead tetraacetate, Ozone, peracids, DDQ and Cr(IV) reagents- Swern Oxidation, Moffattt oxidation, allylic and benzylic oxidation- sommelet reaction- elbs reaction- oxidative coupling of phenols- sharpless asymmetric epoxidation- chemo and regioselectivity in reduction and oxidation, use of XeF_2, SbF_5, VF_5, MoF_6, CF_3OF, SF_4, HF as fluorinating agents

Unit IV **14 Hours**

Chemistry of Polymers:

Type and mechanism of polymerization reaction- Step growth, free radical, addition, ionic, ring opening and group transfer polymerizations- Copolymers- characterization of polymers- methods of measurement of molecular mass and size- stereochemistry of polymers- stereo regularity and its control- Zeigler Natta Catalyst- Gelation and network formation- polymer architecture- configuration and conformation, frictional properties and mechanical properties- glassy and rubbery states- visco electricity- crystallization and melting of polymers- relation between structures, property and performance- manufacture and application of polyolefins, thermoplastics, polyamides, polyesters, polyurethanes, epoxides and industrial polymers.

Unit V **14 Hours**

Heterocyclic Chemistry

Nomenclature of Heterocycles, Replacement and Systematic Nomenclature, Hantzsch – Widman system for monocyclic, fused and bridged heterocycles. Structure, Reactivity, Synthesis and reactions of the following four membered heterocycles – Oxitanes, Azetidines and Thietanes ; Five membered heterocycles – Imidazoles, Pyrazolines, 1,2,4- Triazoles, 1,2,3-Triazoles, Oxadiazole and Thiadiazole; Selenophenes, Tellurophanes and their benzo derivatives; Six membered heterocycles – Pyrones, 1,2,3- , 1,2,4- and 1,2,5 – Triazines , Pyrimidines and Pyrazines; Seven membered heterocycles – Azepines, Oxepines and Thiepines. Fused heterocycles : Indole, Benzofuran , Quinoline, Isoquinolines and Coumarins. Naphthyridines – Synthesis and reactivities.

References

Pavia Lapman Kriz Vyvyan-"***Spectroscopy***"-Ceengage Learning

W Kemp-"***Organic Spectroscopy***"-Palgrave.

J March-"***Advanced Organic Chemistry***"-Wiley.

R O C Norman and A Coxon-"***Modern Synthetic Reactions***"-Chapman and Hall.

M B Smith-"***Organic Synthesis***"-McGraw Hill.

R K Bansal-"***Synthetic Applications in Organic Chemistry***"-Narosa.

Robert M. Silverstein,Francis X. Webster and David Kiemle. "*Spectrometric Identification of Organic Compounds"* **Wiley 2005**

R K Mackie, D M Smith and R A Aitkan-"***Guide Book to Organic Synthesis"-***Longman, 2nd Edn.

R J Simmonds, "***Chemistry of Biomolecules***"-Royal Society of Chemistry.

R J Young-"***Introduction to Polymer Science***"-John Wiley and Sons.

F W Billmayer-"***Text Book of Polymer Science***"- John Wiley and Sons.

G Odian-"***Principles of Polymerization***"- John Wiley and Sons.

J M G Cowie-"***Polymers: Chemistry and Physics of Modern Materials***"-Viva.

K J Saunders-"***Organic Polymer Chemistry***"-Chapman and Hall.

Dr. Jagadamba Singh and Dr. L.D.S Yadav-"***Organic Synthesis***"-Pragathi Prakashan.

Maya Shankar Singh-"***Advanced Organic Chemistry***"-Pearson.

Donald L. Pavia, Gary M. Lampman, George S. Kriz and James R Vyvyan-"***Spectroscopy***"-Cengage Learning.

Ratan Kumar Kar-"***Applications of Redox and Reagents in Organic Synthesis***"-New Central Book Agency.

J. Joule and G. Smith-"***Heterocyclic Chemistry***"-Van-Nostrand, ELBS.

Acheson-"***An Introduction to Heterocyclic Compounds***"-Wiley-Eastern.

Ahluwalia and Parashar-"***Heterocyclicc and carbocyclic chemistry***"- Ane Books.

Jagadanba Singh and Yadav-"***Organic Synthesis***"-Pragati Prakashan Meerut

S.K Ghosh **"Advanced General Organic Chemistry"**Part1and11 New Central BookAgency

PAPER – XII : PHYSICAL CHEMISTRY – III

TOTAL :70 HOURS

UNIT – 1 **14 HOURS**

Reaction Kinetics 1

Review of basic principles: Complex reactions- Reversible, parallel, 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- Lindman- Hinshelwood mechanism and RRKM theories- Fast reaction – relaxation, flow method- flash photolysis- Magnetic and Resonance method.

Theoretical calculation of energy of activation- soling problem involving Ea, E, H and S

UNIT II **14 HOURS**

Reaction Kinetics II

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.

UNIT III **14 HOURS**

Catalysis and Chemical Kinetics:

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 IV **14 HOURS**

Surface chemistry:

Different types of surfaces- Thermodynamics of surfaces- Gibbs adsorption equation and its vertification- surfaces actants and micelles- surface film- surface pressure and surface potential and their measurements and interpretation- Application of Low energy electron- Diffraction and photoelectron- ESCA and Auger Spectroscopy to the study of surfaces.

Adsorption- Langmuir adsorption isotherm- Kinetic and statistical derivation- Multi layer adsorption- Different types- BET theory and Harlein- Jura theory – Measurement of surface area of solids using Langmuir, BET and Harlein-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 Eleyideal mechanism – flash desorption.

UNIT V **14 HOURS**

Colloids:

Structure and stability of colloids, Micelles – The electrical double layer- Eletro kinetic phenomena- zeta potential- electro osmosis- colloids- zeta potential (derivation)- sedimentation potential- streaming potential- donnan membrane equilibrium- Macromolecules- different averages- Methods of molecular mass determination – Osmotic method- sedimentation methods- light scattering methods.

REFERENCE

K.J. Laidler-"***Chemical kinetics***" Pearson Education

S. Glasstone, K.J. Laidler and Eyring-" ***The Theory of rate processe***s"- Mc Graw Hills

J. Rajaram and J.C. Kuriacose- "***Kinetics and Mechanism of chemical transformations***"- Mac Millan India Ltd

Alberty and Silbey- "***Physical chemistry***"- Wiley

G.K. Vemulappally- "***Physical chemistry***"- Prentice Hall of India

P.W. Atkins- "***Physical chemistry***"- Oxford University press

A.W.Adamson- "***The physical chemistry of surfaces***"- 4th edition- Wiley 1982

Alexander and Johnson- " ***Colloid science***"- Oxford University Press

Gavariker- "***Polymer science***" – New age International publishers

SEMESTER – IV

PAPER-XIII ELECTIVES

ELECTIVE PAPER-I (COMPULSARY) - ENVIRONMENTAL CHEMISTRY

TOTAL: 70 HOURS

Unit I **14 HOURS**

Environment-

Concept of environmental chemistry- components of environment- factors affecting environment- segments of environment- formation of physical chemical and biological weathering- composition of soil- process of soil formation. Atmosphere- composition- pressure and temperature changes of troposphere, stratosphere, mesosphere and ionosphere:- Hydrosphere- sea water and river water- composition- dissolved gases- hydrological cycles- biosphere- principles of ecology- shift of ecological activities by human activities- Biogeochemical cycles: C, O, N, S and P cycles- Environmental pollution, pollutant- definition- origin- classification and types of pollution.

Unit II **14 HOURS**

Atmospheric pollution:

Air pollution- sources- industrial- automobiles- fate of air pollutants- chemical reactions in the atmospheric movement of air pollutants- SO_2, NO_x, CO, H_2S, smoke, Hydrocarbons, metal fumes and chlorine- sources and their effect on human and plant system- acid rain- green house effect- smog and photochemical smog- CFC and ozone hole- photochemical reactions in the stratosphere- air pollution control method- Air pollution incidents, Bhopal tragedy

Unit III **14 HOURS**

Soil Pollution:

Effect of fertilizers on soil utilization- agricultural waste- Gobar gas- pesticides and herbicides- classification- reactivity- detection and measurement- thermal and photodecomposition in soil- pesticides residues in soil. Solid waste- classification- sources- disposal. Radioactive waste management- radio nucleides in soil- effect of ionizing radiation- effects on ecosystem- accidents in atomic plants- Chernobyl and Three mile islands disaster- method of radioactive protection

Unit IV **14 HOURS**

Water Pollution:

Sources of water pollution- sewage waste- iron industries- tanneries- detergents. Effect of pollutants- oxygen deficiency- eutrophication- normal level of dissolved oxygen in water for fish growth. Minamatta disaster- treatment f water- water quality criteria for industrial and domestic use Sewage treatment- industrial waste water treatment- drinking water supplies- experimental determination of dissolved oxygen in water- Chemical oxygen demand (COD) and biochemical oxygen demand (BOD)- ISI standard of drinking water.

Unit V **14 HOURS**

Instrumental methods in environmental chemical analysis.

a) Neutron activation analysis **b)** Anodic stripping voltametry **c)** Atomic absorption spectrometry **d)** X-ray fluorescence **e)** Infrared spectroscopy **g)** Chemiluminiscence **h)** Gas chromatography **i)** Ion selective electrodes

REFERENCES

B. K. Sharma and H. Kaur, ***Water Pollution*** Krishna Prakashan Mandir, Meerut

T. H.Y. Tebbut, ***Principles of Water Quality Control*** A. Butterworth-Heinemann***Cleaning our environment - a chemical perspective 2nd edition***, American Chemical Society

J Shapiro ***Radiation Protection*** 4th Ed. Harvard University Press, London

S K Banerjee ***Environmental Chemistry*** Goel Publishing House, Meerut

G. W. Ewing ***Instrumental Method of Chemical Analysis***, McGraw- Hill, New York

L.W. Moore and E. A. Moore, ***Environmental Chemistry*** McGraw Hill Publication, New York

PAPER XIV ELECTIVES

ELECTIVE PAPER I – ORGANIC POLYMERS AND COMPOSITE

TOTAL: 70 HOURS

UNIT- I **14 HOURS**

Introduction to polymer chemistry:

Fundamental concepts of polymer chemistry- development of macro molecular concept – classification of polymers – natural and synthetic polymers- nomenclature of polymers- nomenclature based on source – structure (IUPAC). Polymerization mechanism: mechanism and kinetics of step reaction polymerization- gelation- gelpoint- experimental observation of gelpoint- radical chain polymerization and its mechanism and kinetics- effect of temperature and pressure on chain polymerization- living polymers- coordination polymerization- Ziegler Natta catalyst- polymerization of nonopolar alkene monomers- ring opening polymerization- mechanism of copolymerization.

UNIT- II **14 HOURS**

Characterization of polymers:

Criteria of Polymer solubility- effect of molecular mass on solubility- solubility of crystalline and amorphous polymers- Flory Huggins theory of polymer solution- nature of polymer molecules in solution- viscosity of polymer solution- osmotic pressure- swelling of polymers- fractionation of polymers- measurement of molecular mass: end group analysis, colligative property measurements- concentration dependence of colligative properties- vapour pressure lowering- osmotic pressure measurements- light scattering method- ultra centrifugation- solution viscosity and molecular size- empirical correlation between intrinsic viscosity and molecular size of polymer structures- gel permeation chromatography in the fractionation of polymers.

UNIT-III **14 HOURS**

Structure and Properties of Polymers:

Molecular forces and chemical bonding in polymers- intermolecular forces and physical properties- configuration of polymer chains- crystal structure of polymers- morphology of crystalline polymers- crystallization and melting- strain induced morphology- viscous flow- kinetic theory of rubber elasticity- visco elasticity- mechanical properties of crystalline polymers- crystalline melting point- glassy state and glass transition- factors influencing the glass transition temperature- glass transition temperature and molecular mass- glass transition temperature and plasticizer- glass transition temperature of copolymers- importance of glass transition temperature- properties involving large deformations- properties involving small deformations- property requirements and polymer utilization.

UNIT-IV **14 HOURS**

Polymerization processes:

Polymerization in homogenous and heterogeneous systems- gas phase polymerization, bulk polymerization and polymer precipitation-suspension and emulsion polymerization- solid phase polymerization- Types of polymer degradation: Thermal and mechanical degradation- degradation by ultrasonic waves and by high energy radiation- photo degradation- oxidative and hydrolytic

degradation- biodegradation of polymers- Polymer reactions: basic principles- molecular and chemical groups- reactivity of functional groups- post reactions of polymers- chain extension, branching and cross linking reactions- Polymer analogous reactions: vulcanization- cure reactions- reactions leading to graft and block polytmers- polymer blends- functionalisation of polystyrene.

UNIT-V **14 HOURS**

Polymer processing and commercial polymers:

Plastic technology: moulding, extrusion and other processing methods- additives and compounding- Fiber technology: textiles and fabric 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: Polythylene, poly propylene, polystyrene, polychloroprene, PVC, Teflon, phenol-formaldehyde, urea-formaldehyde resins, polyurethanes, aminoresins, nylons, polyester and caprolactum based polymers.

REFERENCES

F. W. Billmeyer Jr., ***Text book of Polymer Sciences***, Wiley Intersciences

George Odian, ***Principles of Polymerization, 3rd ed***. John Wiley and Sons

P. J. Flory, ***Principles of Polymer Chemistry***, Cornel University Press, London

J. A. Brydson, ***Rubber Chemistry***, Applied Sciences London

F. Rodrigues, ***Principles of Polymer Systems***, McGraw Hill Boom Company

J. M. C. Cowie, ***Polymer Chemistry and Physics of Modern Materials***, International Text Book Company

J. A.Bridesson, ***Plastic Materials***, Newness Butterworth

R. J. Young, ***Introduction to Polymer Sciences***, John Wiley and Sons

K. J .Saunders, ***Organic Polymer Chemistry***, Chapman and Hall

V R Gowrikar and others, ***Polymer Science***, new age.

Elias, ***Macro Molecules***, Plenum Press.

I M Campbell***, Introduction to Synthetic Polymers***, Oxford Scientific Publications.

H R Allocock, F W Lampe***, Contemporary Polymer Chemistry***, Pearson

R B Symour and E C Carraher, ***Polymer Chemistry*** *Marcel Dekker, Inc,* ***,*** *New York*

G S Misra, ***Introduction to Polymer Chemistry***, New Age

Naren, ***Polymer as Aids in Organic Chemistry*** Academic Press, London.

Deeksha Dave, S. S. Katewa ***Text Book of Eenvironmental Studies*** Ceengage

ELECTIVE PAPER - II

ELECTROCHEMISTRY AND INDUSTRIAL CATALYSIS

TOTAL – 70 HOURS

UNIT – I **14 hours**

Electrochemistry

Electrochemical cells- Daniel cell- Leclanche cell- and dry cell- Storage of Electricity- Lead acid battery- principle and construction- Fuel cell- H_2-O_2 cell- Working principle- Modern developments in the application of electrochemical cells- Silver oxide and lithium cells- Nickel- Cadmium batteries- Solid electrolyte cells.

UNIT- II **14 hours**

Photo electro chemistry:

Effect of radiation of light on matter- photo physical phenomena-photovoltaic effect- Solar cell-construction and working principle- Storage of solar energy- Photo assisted electrolysis of water.

UNIT – III **14 hours**

Industrial electro chemistry:

Electro organic synthesis-Kolbes synthesis- Lead tetra ethyl synthesis- Adiponitrile synthesis-Oxidation and reduction of hydrocarbons- Reduction of nitro compounds-Electroinorganic synthesis of fluorine, chlorates, perchlorates- Polorography-Amperometry.

UNIT – IV **14 hours**

Industrial catalysis:

Theories of adsorption-BET theory, Statistical derivation and its application- Adsorption isotherms and isosters-their significance- Determination of heat of adsorption- Kinetics of heterogeneous catalysis-Absolute rate theory of catalysis- Energy profile diagram in heterogeneous catalysis.

Electronic factors in catalysis by metals and semiconductors- Cooperative electronic inter action in catalysis- Preparation of solid catalyst and supports- Preparation of supported catalyst- Silica, silica-alumina, zeolite, carbon catalysts-selectivity. Polymer support and heterogenisation-catalytic deactivation-poisoning and fouling.

UNIT –V **14 hours**

Catalysis by organometallic compounds:

Oxidative addition, reductive elimination and Insertion reactions- Wilkinson's catalysts

Some typical catalytic processes- Olefein hydrogenation- Wacker process- Zeigler Natta process-Monsanto process- Fischer- Tropsch process- Cracking of petroleum.

REFERENCES

S. Glasstone **Introduction to Electrochemistry,** Affiliated East-west Press Pvt Ltd (1996)

Bard A. J. and Faylkner L.R **Electrochemical methods**, John Wiley

Ed Lindin **Hand book of Batteries and Fuel cells** McGraw-Hill

Bockris and Reddy- "***Modern electrochemistry***"- Springer 2nd Edition volumes 1, 2A and 2B

H.H Willard, LL Merrit, J.A Dean **Instrumental methods of Analysis,**. Van Nostrand

J. M Betty,Ed Bruce, E Leach **Applied Industrial Catalysis**, Academic Press

Ed Pearce, W.R.Patterson **Catalysis and Chemical Processes**, Blackie and Sons

G Somarajan **Principles of Surface Chemistry** Prentice Hall

F. A. Cotton and G. Wilkinson, ***Advanced Inorganic Chemistry***, 5th ed., J. Wiley

A. W. Parkins and R C Pollar **An Introduction to Organo metallic Chemistry:** Macmillan

ELECTIVE PAPER - III

CERAMICS AND COMPOSITES

UNIT-I **14 HOURS**

Ceramic materials: Definition of ceramics-

Traditional and new ceramics- structure of ceramics- atomic interactions and types of bonds- phase equilibria in ceramic systems- one component and multi component systems- use of phase diagrams in predicting material behavior- electrical, magnetic and optical properties of ceramic materials.

UNIT II **14 HOURS**

Crystalline and Non crystalline ceramic materials:

Chemical reactions at high temperatures and processing of ceramics- high temperature materials- crystalline ceramic materials- oxide, carbide, nitride, graphite and clay materials and their structures- polymorphism- Non crystalline ceramic materials- structure and structural requirements for stability- mode of formation- silicate and non silicate glasses- hydrogen bonded structures.

UNIT III **14 HOURS**

Nano technology:

Nano materials- definition- nano structures- self assembly- nano particles, methods of synthesis- sol-gel process, colloids, hydrolysis of salts and alkoxides, precipitation condensation reactions, electro kinetic potential and peptization reactions- gelation network- xerogels, aero gels- drying of gels- chemical modification of nano surfaces- applications of sol- gel process, sol gel coating, porous solids, catalysts, dispersions and powders.

UNIT IV **14 HOURS**

Materials for special purposes:

Production of ultra pure materials- zone refining, vacuum distillation and electro refining.

Ferro electric and piezo electric materials:

General properties- classification of ferro electric materials- theory of ferro electricity- ferro electric domains- applications. Piezo electric materials and applications. Metallic glasses, preparation, properties and applications.

Magnetic materials-

ferri and ferro magnetism- metallic magnets- soft, hard and super conducting magnets- ceramic magnets- low conducting and super conducting magnets.

Super conducting materials:

Metallic and ceramic super conducting materials- theories of super conductivity- Meissner effect- high temperature super conductors, their structure and applications.

UNIT V **14 HOURS**

Composite materials

Definition and classification of composites- fibers and matrices. Composite with Metallic matrices- Metal matrix composite processing, solid and liquid state processing, deposition. Ceramic matrix

composite materials- Introduction- processing of ceramic matrix composites- mixing and pressing, liquid state processing of ceramic matrix composites- mixing and pressing, liquid state processing, sol-gel processing, vapour deposition technique- Interfaces in composites- mechanical and micro structural characteristics.

Polymer composites-

Role of fibre and matrix in improving properties-bonding between fiber and matrix- critical fibre length in short fibre composites- failure mechanism in composites- composite fabrication techniques- open mould process, hand lay up, vacuum bag moulding, centrifugal casting.

Application of composites.

REFERENCES

W D Kingery, H K Dowen and R Duhlman- ***"Introduction to Ceramics"*** - John Wiley.

F H Nortion- ***"Elements of Ceramics"*** Addison-Wesley Pub. Co**.**

C J Brinker and G W Sherer- ***"Sol-Gel Science, The Physics and Chemistry of Sol-Gel processing"*** - Academic Press, Newyork,

A G Guy- ***"Essentials of material Science"*** - McGraw Hill.

M J Starfield and Shrager- ***"Introductory Materials Science"*** - McGraw Hill.

V Raghavan- "***A First Course in Material Science***" - Prentice Hall Pvt Ltd, New Delhi.

J F Shackelford- ***"An Introduction to Materials Science for Engineers***" McMillan Pub. Co. New York.

W F Smith- ***"Foundation of Materials Science & Engineering***" - McGraw Hill Book Co. 2000

M W Barsoum- ***"Fundamentals of Ceramics"*** - McGraw Hill Book Co. 1997.

S K Hajra Chaudhary- ***"Material Science and Engineering"*** – Indian Book Dist Co. Culcutta.

Sharpe R S- ***"Research Techniques in Non Destructive Testing, Vol II***" – Academic Press, New York, 1973.

J Kraut Kramer and H Kraut Kramer- ***"Ultrasonic Testing of Materials***" – George Allen & Union Ltd, London, 1969.

"***Analytical Techniques for Thin Films in Treatise on Material Science & technology***, Vol 27" – Acad. Press Inc., N.Y,1991.

S V Subramanyan and E S Rajagopal- "***High Temperature Super Conductors***" – Wiley Eastern Ltd. 1988.

M Tinkham- "***Introduction to Super Conductivity***" – McGraw Hill, Kogakusha Ltd, 1975.

A V Narlikar and S N Edbote- ***"Super Conductivity and super conducting Materials***" – South Asian Pub., New Delhi 1983.

Dekker- ***"Electronic Engineering Materials***" – A J Prentice Hall mof India Pvt.Ltd. 1985.

C M Srivastava and C Srinivasan- ***"Science of Engineering Materials***" – Wiley Eastern Ltd, 1987.

Azaroff and Brophy- "***Electronic Process in Materials***" – McGraw Hill, 1985.

K K Chowla- "***Composite Materials"*** – Springer-Verlag N Y 1987.

F R Jones- "***Hand Book of Polymer Fibre Composites***" – Longman Scientific & Tech, 1994.

ELECTIVE PAPER - VI
COMPUTATIONAL CHEMISTRY

UNIT I- **14 Hours**

Molecular mechanics

Perspective- basic principles-Developing force field- The stretch energy- The bending energy- The torsional energy- The Vander walls energy- The electrostatic energy- Cross terms- Parametrising the force field- Calculation using the force field - Geometries and energies of Small to medium sized molecules- Polymers- transition states-MM in organic synthesis-Molecular mechanics and Monte Carlo simulations- Geometries and frequencies calculated by MM -Strength and weakness of MM-Hybrid force field Electronic structure methods.

UNIT II **14 Hours**

Introduction of Quantum mechanics in Computational Chemistry-

Perspective- The development of quantum mechanics-The Born Oppenheimer approximation-Schrödinger equation- Koopman's theorem- Restricted and unrestricted Hartree- Fock models-Application of the Schrödinger equation to chemistry by Huckel- Hybridisation-matrices and determinants- simple Huckel theory-Application-The nodal properties of MOs – Stability indicated by energy levels and aromaticity. Extended Huckel method.

UNIT III **14 Hours**

Abinitio Calculation

Perspective- The basic principles of the abinitio method. Approximation methods- Self-Consistent field theory- The energy of a Slater determinant- Hartree- Fock equation- Basis sets- Slater and Guassian type orbitals-Classification of basic sets- Minimum basis set- Split valence- diffused and polarization and correlation consistent basis sets- post HF calculation- Application- Geometry optimization ,Frequency calculation and transition state optimization of simple systems-Strength and weakness-Configuration interaction, Moller- plesset perturbation theory and Coupled cluster methods-(qualitative study only)- -

UNIT IV **14 Hours**

Semi Empirical Method

Perspective-The basic principle of SCF-SE methods- Neglet of diatomic differential overlap approximation(NDDO)- Intermediate Neglet of differential overlap approximation(INDO)-

Complete Neglet of differential overlap approximation(CNDO)- Parameterization- Modified Intermediate Neglet of differential overlap (MINDO)-Modified NDDO &MNDO models- Austin model1(AM1) application- Geometry optimization ,Frequency calculation and transition state optimization of simple systems Strength and weakness

UNIT V **14 Hours**

Density Functional Calculation

Basic principle –Orbital free density functional theory- Kohn-sham theory -Reduced density matrix methods-

Local density approximation application- Higher ordergradient or meta-GGA methods-Hybrid or hyper-GGA methods- Performance and properties of density functional methods- Geometry optimization ,Frequency calculation and transition state optimization of simple systems- Strength and weakness

REFERENCES:

Errol Lewars *'**Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics'*** Spriger India

I.N Levine ***Quantum Chemistry***, Prentice Hall of India Vth edition

Tamas Veszpremi and Miklos Feher ***Quantum Chemistry: Fundamentals to applications*** Springer India

David C Young, ***Computational Chemistry:. A Practical Guide for Applying Techniques to Real World Problems*** Wiley Interscence

P.W. Atkins, ***Molecular Quantum Mechanics***. Oxford University Press

G. H. Grant and W. G. Richards ***Computational Chemistry*** Oxford University Press

INORGANIC PRACTICALS II

(IIIrd and IVth Semester)

Time: 125 Hours.

1. Quantitative separation of binary mixtures and estimation of one of the component by gravimetric method.

   Cu(II), Ni (II), Fe(III), Mg(II), Ap(III), Ca(II), Ba(II) & Zn (II)

2. Analysis of Ores and Alloys.

   a) Analysis of Dolomite – insoluble residue by gravimetric and Ca and Mg by complexometric methods.

   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. Iron exchange separation of binary mixtures such as those of Zn(II), Mg(II) and Co(II), Ni(II)

4. Preparation of the following complexes and checking the purity by metal content analysis.

   a) Potassium trioxalatoferrate (II)

   b) Potassium hexathiocyanatochromate(III)

REFERENCES

G. H. Jeffrey, J.Bassette, J. Mendham and R.C. Denny, ***'Vogels Text Book of Quantitative Inorganic Analysis***' ELBS Publication, London 1997

D.M.Adams and J.B Raynor '***Advanced Practical Inorganic Chemistry'*** CRC Press, New York

W.L.Jolly, '***Preparative Inorganic Reactions'*** Interscience Publishers, New York

PAPER-V

ORGANIC PRACTICALS-II

(IIIrd and IVth Semester)

TIME:125 HOURS

1. Quantitative Analysis: Determination of (a) equivalent weight of a carboxylic acid, (b) reducing sugars using Fehling's solution,(c) phenol, salicylic acid, aspirin and aniline using bromate-bromide mixture, (d) ketomethyl group in water soluble ketones such as MEK and acetone, (g) iodine and saponification values of vegetable oils and (h) nitrogen by kjeldahl method and sulphur gravimetrically(i)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-tribromoaniline→tribromobenzene.
   c) Methyl Orange: Aniline→sulphanilic acid→methyl orange.
   d) p-Aminobenzene: Aniline→diazoaminobenzene→p-aminoazobenzene.
   e) N-Acetyl anthranilic acid: o-Toluedine→o-methylacetanilide→N-actylanthranilic acid.
   f) P-Chlorobenzoic acid: p;Toluedine→p-chlorotoluene→p-chlorobenzoic acid.
   g) M-nitroaniline: Nitrobenzene→m-dinitrobenzene→m-nitroaniline.
   h) Benzil: Benzaldehyde→Benzoin→-Benzil.
   i) M-Nitrobenzoic acid: Methyl benzoate→m-nitromethylbenzoate→m-nitrobenzoic acid.
   j) Benzanilide: Benzophenone→Benzophenoneoxime→benzanilide.
3. Extraction of natural products: Caffeine from tea leaves, Chlorophyll(Soxhlet extraction), citral from lemon grass(steam distillation), Caesin from milk.
4. Practical application of TLC: Identification of food colors, amino acids, sugars, terpenoids, alkaloids, steroids, flavanoids, organochloropesticides, organo phosphorous pesticides, carbamate pesticides, Indole acetic acid.

REFERENCES

A I Vogel- ***"A Text Book of Practical Organic chemistry***" – Longman.

"Elementary Practical Organic Chemistry, Part 3 Quantitative Organic Analysis"- Longman.

F G Mann and B C Saunders- ***"Practical Organic Chemistry***"- Longman.

P R Singh, D c guptha and K S Bajpai- ***" Experimental Organic Chemistry Vol I & II"***.

Sadasivam S and Manickam A- ***"Biochemical Methods"*** – New Age International Publishers.

J B Harborne- ***"Phytochemical methods"*** - Chapman and Hall, London.

Joseph Sharma, Gunter Zweig- ***"TLC and LC analysis of International importance Vol VI & VII"*** – Academic Press.

PAPER- VI

PHYSICAL PRACTICALS-II (III & IV SEMESTER)

TIME: 125 HOURS

A minimum of 30 experiments covering all units

1. **Chemical Kinetics**

Acid hydrolysis of ester (methyl acetate of ethyl acetate) – Determination of the given acids

Acid hydrolysis of ester-Determination of Arhenius parametrs

Saponfication of ethyl acetate-Determination of specific reaction rate

Iodination of acetone in acid medium-Determination of order of reation with respect to iodine and acetone

2. **Adsorption**

Verification of Freundlich and Langmuir adsorption isotherms- charcoal- acetic acid system

Determination of the concentration of a given acetic acid solution using the isotherms

Same experiment using charcoal- oxalic acid system

3. **Conductivity Experiments**

Equivalent conductance of weak acid- verification of Ostwald's dilution law – calculation of dissociation constant

Equivalent conductance of strong electrolysis (KCI) Verification of Onsagar equation.

Activity coefficient of Zn in 0.002m $ZnSO_4$ using Debye-Huckel limiting law.

Solubility product of sparingly soluble salts (AgCl, $BaSO_{4)}$

Conductance titrations HCl vs NaOH, (HCl+HAc) vs NaOH $AgNO_3$ vs KCl

4. **Polarimetry**

Determination of specific and molar optical rotations of glucose, fructose and sucrose

Determination of the concentration of a glucose solution

Inversion of cane sugar in presence of HCl- Study of the kinetics

Determination of specific rate of the reaction

Determination of the concentration of HCl

5. **Spectrophotometry**

Verification of Beer-Lamberts law

Determination of equilibrium constants of acids- base indicators.

Determination of concentration of a solution of $K_2Cr_2O_7$ (or $KMnO_4$)

Simultaneous determination of Mn and Cr in a solution of $KMnO_4$ and $K_2Cr_2O_7$

Investigation of complex formation between Fe (III) and Thiocyanate.

6. **Chromatography:**

Separation of inorganic ions by paper chromatography(Fe, Co, Mn and Ni)- ion exchange chromatography- Determination of the concentration of a salt solution by ion exchange chromatography- Determination of the composition of a solution containing an acid and its salt.

7. **Computer Applications in Chemistry:**

Computer programming in chemistry: writing of computer programmes in C languages for problems of chemical interest and their executions. Programming examples to handle the following numerical methods in chemistry - least square fit, solutions of simultaneous equations, polynomial equation fitting, matrix inversion and diagonalisation and numerical differentiation and integration - Programming for organic, physical and inorganic chemistry Splines and data smoothing - Elements of parallel processing and its use in chemistry - Least square fit, graphics, kinetics,(Monte Carlo simulation of kinetics, potentiometric titrations and end point locations, fitting curves and floating functions). Simulation studies - Drawing of chemical structures – Chemdraw / Chemsketch / Hyperchem.

REFERENCES

A. Findlay and J. A. Kitchener, ***Practical Physical Chemistry***, Longman

F. Danieles and J. H. Mathews, ***Experimental Physical Chemistry***, Longman

A. M. James, ***Practical Physical Chemistry***, J. A. Churchil

H. H. Willard, L. L .Merit and J. A. Dean***, Instrumental Methods of Analysis***" Affiliateed East West Press

D. P. Shoemaker and C. W. Garland, ***Experimental Physical Chemistry***, McGraw Hill

K. V. Raman, ***Computers in Chemistry***, McGraw Hill

Wickens et al. ***Introduction to Computer Programming for Chemistry***, Allyn and Bacon, London

K. B. Wiberg, ***Computer Programming for Chemists***, Benjamin Inc.

Mattson, ***Computers in chemistry and instrumentation, Vol. 1-5***, Marcel Decker

K. J. Johnson, ***Numerical Methods in Chemistry***, Marcel Decker.

Sd/-
Dr.Zeinul Hukuman.N.H,
Chairman,BOS Chemistry(PG)