Shrimathi Devkunvar Nanalal Bhatt Vaishnav College (Autonomous)

Re-accredited at "A" Grade by NAAC

M.Sc. DEGREE COURSE IN CHEMISTRY

Choice Based Credit System

Syllabus Submitted to the University of Madras for Approval

REGULATIONS

(Effective from the academic year 2016-2017 onwards)

1. Eligibility for Admission

Candidate who has passed the under-mentioned degree examinations of this University or an examination of other institution recognized by this University as equivalent thereto provided they have undergone the course under 10+2+3, shall be eligible for admission to the M.Sc. Degree Course.

(a) B.Sc. in Chemistry

2. Duration of the Course

The Course duration shall be **Two** years consisting of four semesters. In order to be eligible for the award of the degree the candidate shall successfully complete the course in a maximum period of five years reckoned from the date of enrolment for the first semester of the course.

3. Structure of the Course and Evaluation Pattern

The duration of external examination for theory and practical subjects shall be 3 hours. The maximum mark for each theory is 100 with 25 for Continuous Internal Assessment (CIA) and 75 for End Semester Examination (ESE). The distribution of internal marks for theory papers shall be: Two best tests out of Three (each test 10 marks, therefore (10x2=20) 20 marks, Quiz /Assignment/Seminar - 5 marks. The maximum mark for each practical is 100 with 40 for Continuous Internal Assessment (CIA) and 60 for End Semester Examination (ESE). The distribution of internal marks for practical papers : Practical Internal marks 8 best test (8x5=40) 40 marks and Practical External marks ,out of 60 marks, record-5 marks,viva-voce-10 marks and exam 45 marks. For project work the marks assigned shall be

Internal	Two	best	out	of	three	
presentati	ons	(2x 10)=20)			20 marks
External I	60 marks					
External Viva-voce						20 marks

For the conduct of External Examinations in Practical subjects the Controller of Examination of the college will appoint one external examiner, one internal examiner who shall normally be the concerned practical in-charge. The Controller of Examination will give the question bank. The examiners will conduct the examinations and award the marks on the same day and forward to the Controler of examinations. The head of the department will coordinate and provide the laboratory and other facilities for conducting the examination.

Project work shall be carried out individually in an R&D section of any Industry or in the Institute in which the candidate is studying. The Project Work/Dissertation report shall be submitted through the guides/supervisors to the Head of the Department and then to the Controller of Examinations not later than 31st May/31st December. If he/she fails to submit the Project Work/Dissertation within the stipulated date for a particular semester, he/she may be permitted with the approval of the Head of the Department to submit the Project Work/Dissertation report during the succeeding semesters, within the maximum period of **FIVE** years from the date of admission to the first semester. Project/Dissertation evaluation and Viva-Voce shall be conducted by one external examiner and one internal examiner who shall normally be the project guide.

List of courses, Scheme of evaluation and their associated credits are given below:

M.Sc., DEGREE COURSE IN CHEMISTRY

SEMESTER-I

S.N	SUBJECT	papers	TITLE OF THE	С	LH/W	CIA	ESE	Т
0			PAPER					
1	Core T-I	1	Organic Chemistry-I	4	6	25	75	100
2	C ore T-II	1	Inorganic Chemistry-I	4	6	25	75	100
3	Core T-III	1	Physical Chemistry-I	4	6	25	75	100
4	Elective-I	1	Polymer Chemistry	3	4	25	75	100
5	Core P -I	1	*Organic Chemistry	4	8	40	60	100
			Practical -I					
6	Soft Skill	1	Essentials of Spoken	2		20	80	100
			and Presentation skills					
		6		21	30			
TOTAL MARKS MAJOR -400 ; ELECTIVE -100								

CIA – Continuous Internal Assessment ESE – End Semester Examination

LH/W-Lecture hour/week; C-Credits

SEMESTER-II

S.NO	SUBJECT	papers	TITLE OF THE PAPER	C	LH/ W	CIA	ESE	Т
1	Core T-IV	1	Organic Chemistry-II	4	5	25	75	100
2	Core T-V	1	Inorganic Chemistry-II	4	5	25	75	100
3	Core T-VI	1	Physical Chemistry-II	4	5	25	75	100
4	Elective-II	1	Nano Chemistry	3	4	25	75	100
5	Core P-II	1	*Inorganic Chemistry Practical-I	4	8	40	60	100
6	NME-I	1	Chromatographic Techniques	3	3	25	75	100
7	Soft Skills	1	Spoken and Presentation skills-Advanced level	2		20	80	100
		7		24	30			
	TOTAL MARKS MAJOR -400 ; ELECTIVE -100 ;NME-100							

CIA – Continuous Internal Assessment ESE – End Semester Examination

LH/W-Lecture hour/week ;C-Credits

* Practicals will be conducted at the end of even semester

S.NO	SUBJECT	papers	TITLE OF THE PAPER	C	LH/W	CIA	ESE	Т
1	Core T-VII	1	Organic Chemistry- III	4	5	25	75	100
2	Core T-VIII	1	Inorganic Chemistry- III	4	5	25	75	100
3	Core T-IX	1	Physical Chemistry- III	4	5	25	75	100
4	Elective-III	1	Electro Chemistry	3	4	25	75	100
5	NME-II	1	Environmental Chemistry	3	3	25	75	100
6	Core P -III	1	*Inorganic Chemistry Practical - II	4	8	40	60	100
7	Internship	1	Internship	2		-	-	-
8	Soft Skills	1	Personality enrichment	2		20	80	100
		8		26	30			
	TM MAJOR -400 ; ELECTIVE -100 ;NME-100							

SEMESTER-III

CIA – Continuous Internal Assessment ESE – End Semester Examination

LH/W-Lecture hour/week ; C-Credits

SEMESTER-IV

S.NO	SUBJECT	papers	TITLE OF THE PAPER	С	LH/	CIA	ESE	Т
					W			
1	Core T -X	1	Organic Chemistry-IV	4	5	25	75	100
2	Elective -IV	1	Research Methodology	3	4	25	75	100
3	Elective-V	1	Analytical Techniques	3	4	25	75	100
			in Chemistry					
4	Core P-IV	1	*Physical Chemistry	4	8	40	60	100
			Practical					
5	Project	1	Project	4	9	20	80	100
6	Soft Skills	1	Life and managerial	2		20	80	100
			Skills					
		6		20	30			
	TM MAJOR -200 ; ELECTIVE 200							

CIA – Continuous Internal Assessment ESE – End Semester Examination

LH/W-Lecture hour/week,C-Credits

	MARKS	CREDITS
MAJOR(THEORY+PRACTICAL)/ELECTIVE/NME/PROJECT		
	2200	81
SOFT SKILLS/INTERNSHIP		
	400	10
TOTAL		
	2600	91

• Practicals will be conducted at the end of even semester

CREDITS DISTRIBUTION

Course Type	Course	Credits	Total Credits
Core (Theory)	10	4	40
Core (Practical)	4	4	16
Core (Project)	1	4	4
Elective	5	3	15
Internship	1	2	2
Skill based courses	4	2	8
Non-major elective	2	3	6
Total			91

PROCEDURE FOR INTERNAL MARKS

Theory	Internal Marks (25)	
	Distribution	
	Tests	= 20
	= 5	

Practical	Internal Marks	(40)	
	Distribution		
	Tests		= 40

Pattern of question Paper

THEORY/ NON MAJOR ELECTIVE

Time 3 hours

Max Marks 75

Part – A

Ten Out of Twelve questions. (10 x 2 = 20 Marks)

At least two questions from each unit and not more than three questions from each unit.

Part –B

Five Out of Seven questions. $(5 \times 5 = 25 \text{ Marks})$

At least one question from each unit and not more than two questions from each unit.

Part –C

Three Out of Five questions. $(3 \times 10 = 30 \text{ Marks})$

One question from each unit

PRACTICAL

Time: 6 Hours

Max: 60 Marks.

6. Requirements for proceeding to subsequent semesters

- 1) Candidate shall register their names for the First Semester Examination after the admission in the M.Sc (Chemistry) Course.
- 2) Candidates shall be permitted to proceed from the first semester up to the final Semester irrespective of their failure in any of the Semester Examinations subject to the condition that the candidate should register for all arrear subjects of earlier semesters along with current (subject) semester subjects.
- 3) Candidates shall be eligible to proceed to the subsequent semester, only if they earn sufficient attendance as prescribed thereof by the University/College from time to

time.

Provided in case of candidate earning less than 50% of attendance in any one of the semester due to any extraordinary circumstance such as medical grounds, such candidates who shall produce medical certificate issued by the Authorized Medical Attendance (AMA), duly certified by the Principal of the College, shall be permitted to proceed to the next semester and to complete the course of study. Such candidate shall have to repeat the missed semester by rejoining after completion of final semester of the course, after paying the fee for the break of study as prescribed by the University/College from time to time.

4) Candidates earning less than 65% and more than 50% will NOT be considered Eligible for the current semester. They will have to write the current semester papers as Arrears in the following semester after paying the condonation fees.

7. Passing Requirements

- 1) There shall be no passing minimum for Internal.
- 2) For all subjects (Theory/Practical/Project) the passing requirement is as follows: candidate secures not less than 50% of marks in End Semester Examination (ESE) and not less than 50% in aggregate of the total internal and external marks.
- 3) A candidate who passes in all subjects and in the project work earning 91 credits(including Soft Skills and Internship) within the maximum period of five years reckoned from the date of admission to the course shall be declared to have qualified for the degree.
- 4) Grading shall be based on overall marks obtained (Internal + External)

8. Classification of successful candidates

- (a) A Candidate who qualifies for the Degree and secures CGPA between 9.0 10.0 shall be declared to have passed the examination in FIRST CLASS - EXEMPLARY provided he/she has passed the examination in every subject he/she has registered as well as in the project work in the first appearance.
- (b) A Candidate who qualifies for the Degree and secures CGPA between 7.5 − 8.9 shall be declared to have passed the examination in FIRST CLASS WITH DISTINCTION provided he/she has passed the examination in every subject he/she has registered as well as in the project work in the first appearance.
- (c) A candidate who qualifies for the degree as per the regulations for passing requirements and secures CGPA between 6.0 7.4 shall be declared to have passed the examination in **FIRST CLASS**
- (c) All other successful candidates shall be declared to have passed in **SECOND CLASS**.

(d) Only those candidates who have passed all the papers including practical and project work in the first appearance shall be considered for the purpose of **RANKING**.

9. Procedure in the event of failure

- a) If a candidate fails in a particular subject (other than Project work) he/she may reappear for the External examination in the subject in subsequent semesters and obtain passing marks.
- b) In the event of failure in Project Work, the candidate shall reregister for Project Work and redo the Project Work in a subsequent semester and resubmit the dissertation afresh for evaluation. The internal assessment marks shall be freshly allotted in this case.

10. Attendance

A candidate who has attendance of less than 75% overall in a semester shall not be permitted to take the External examination. However, it shall be open to the Academic Head/Principal to grant exemption to a candidate if he/she possess 65% or more attendance but less than 75% after paying the required condonation fee to the University for valid reasons and such exemptions should not under any circumstances be granted for attendance below 65%. Candidates who have less than 65% and those who have less than 75% but have not got the exemption as above, has to repeat the semester from the next academic year.

11. Grading System

The term grading system indicates a SEVEN (7) point scale of evaluation of the performances of students in terms of marks obtained in the Internal and External Examination, Grade points and letter grade.

Marks and Grades:

Conversion of Marks to Grade Points and Letter Grade (Performance in a Course / Paper)

Range Of Marks	Grade Points	Letter Grade	Description
90-100	9.0-10.0	0	Outstanding
80-89	8.0-8.9	D+	Excellent
75-79	7.5-7.9	D	Distinction
70-74	7.0-7.4	A+	Very Good
60-69	6.0-6.9	А	Good
50-59	5.0-5.9	В	Average
00-49	0.0	U	Re-appear
ABSENT	0.0	AAA	ABSENT

For a Semester :

GRADE POINT AVERAGE [GPA] = $\sum_{I} C_{I} G_{I} / \sum_{I} C_{I}$

Sum of the multiplication of grade points by the credits of the courses

GPA = -----

Sum of the credits of the courses (Passed) in a semester

For the entire programme:

CUMULATIVE GRADE POINT AVERAGE [CGPA] = $\sum_{n} \sum_{I} C_{ni} G / \sum_{n} \sum_{i} C_{ni}$

Sum of the multiplication of grade points by the credits of the entire programme

CGPA= -----

Sum of the credits of the courses(Passed) of the entire programme

 C_i - Credits earned for course 'i' in any semester

 G_i - Grade point obtained for course 'i' in any semester

n' - refers to semester in which such courses were credited

ССРА	Grade	Classification Of Final Result
9.5-10.0	O+	First Class - Exemplary *
9.0 and above but below 9.5	0	
8.5 and above but below 9.0	D++	First Class with Distinction *
8.0 and above but below 8.5	D+	
7.5 and above but below 8.0	D	
7.0 and above but below 7.5	A++	
6.5 and above but below 7.0	A+	First Class
6.0 and above but below 6.5	А	
5.5 and above but below 6.0	B+	Second Class
5.0 and above but below 5.5	В	

* The candidates who have passed in the first appearance and within the prescribed semester of the M.Sc(Chemistry) Programme (Core and Elective courses alone) are eligible.

12. Pattern of question Paper

THEORY/ NON-MAJOR ELECTIVE

Time 3 hours

Max Marks 75

Part – A

Ten Out of Twelve questions. (10 x 2 = 20 Marks)

At least two questions from each unit and not more than three questions from each unit.

Part –B

Five Out of Seven questions. $(5 \times 5 = 25 \text{ Marks})$

At least one question from each unit and not more than two questions from each unit.

Part –C

Three Out of Five questions. $(3 \times 10 = 30 \text{ Marks})$

One question from each unit

PRACTICAL

Time: 6 Hours

Max: 60 Marks.

DEGREE OF MASTER OF CHEMISTRY (M.Sc.)

SYLLABUS IN DETAIL

(Effective from the academic year 2016-2017 onwards)

Core Major Theory- I – Organic Chemistry - I

Credits -4

Max.Marks-75

Objectives

This course aims to explain basic concepts in stereo chemistry and conformational analysis of organic molecules. In addition, the reaction mechanism and synthetic application of aliphatic and aromatic substitution reaction in organic synthesis will be discussed in detail.

Unit I: Stereochemistry:-

Introduction to optical activity and chirality, , prochiral carbons. Configuration and conformational isomers. Absolute configuration-enatiomers- R, S nomenclature.

Steroisomerism due to molecular dissymmetry-allenes, biphenyls, spiro compounds, trans cyclooctene and cyclononene and molecules with helical structures enantiotopic, homotopic and diastereotopic hydrogens in compounds up to ten carbons only. Stereo specific and stereo selective reactions. Inter conversion of Sawhorse, Newman and Fischer projections. Molecules with more than one asymmetric center -definition of diasteroisomerconstitutionally symmetrical, unsymmetrical chiral compounds E.g. erythro and threo compounds.

Geometrical isomerism. E, Z nomenclature of olefins, geometrical and optical isomerism (if shown) of disubstituted cyclopropane, cyclobutane and cyclopentanes.

Unit II: Conformational analysis:-

Conformation of some simple, 1, 2-disubstituted ethane derivatives. Conformational analysis of disubstituted cyclohexanes and their stereo chemical features [cis, trans and optical isomerism (if shown) by these derivatives]. Conformation and reactivity of substituted cyclohexanols (oxidation and acylation), cyclohexanones (reduction involving selectrides) and cyclohexane carboxylic acid derivatives (esterification and hydrolysis).Conformational analysis of cyclohexenes. Conformation and stereochemistry of cis and trans decalin and 9-methyl decalin.

Unit III: Nucleophilic Substitution reactions:-

Aliphatic Nucleophilic substitution- $S_N 1$, $S_N 2$ and $S_N i$ mechanism - Nucleophile and leaving groups Stero chemistry and Ion pairs. Neighbouring group participation – by Aryl group, O, N, S halogens, single, double and triple bonds. Reactivity, structural, solvent and steric effects. Substituent effect on carbocations – cyclopropyl and carbonyl cations. Substitution in norbornyl system and at bridgehead carbon. Substitutions by ambident nucleophiles such as CN, NO₂, phenoxide and allkylation using dianion (EAA), acylation and alkylation of active methylene compounds.Nucleophilic substitution at carbon which is doubly bonded to oxygen and nitrogen - alkylation and acylation of amines, halogen exchange, Von-Braun reaction. Claisen and Dieckmann condensations.

Aromatic nucleophilic substitution - methods of generation of benzyne intermediate and reactions of aryne intermediates. Nucleophilic substitution involving diazonium ions. Aromatic nucleophilic substitution of activated halides. Ziegler alkylation. Chichibabin reaction. Hammet equation. Derivation and free energy relationship, simple problems. Taft equation

Unit IV: Electrophilic substitution reactions:-

Arenium ion mechanism. Orientation and reactivity (ortho, meta and para directing groups) of nitration, halogenation, alkylation, acylation and diazonium coupling. Formylation reactions - Gatterman, Gatterman-Koch, Vilsmeyer-Hack & Reimer-Tieman Reaction. Synthesis of di & tri substituted benzenes (symmetrical tribromobenzene, 2-amino-5-methylphenol, 3-nitro-4-bromobenzoicacid, 3, 4-dibromonitrobenzene, 1, 2, 3 - trimethylbenzene) starting from benzene or any mono substituted benzene.

Unit V: Terpenoids and Steroids:-

Flavones, isoflavones, anthocyanins (Synthesis of parent and simple alkyl or aryl substituted derivatives are expected). Synthesis of carotenoids, licopenes and Vitamin A1 (Reformatsky and Wittig reaction methods only).

Structural elucidation of cholesterol (by chemical degradation). Conversion of cholesterol to progestrone, esterone and testosterone.

Text Books:-

- 1. E. Eliel, S.H.Wilen and L.N.Mander, 1994, Stereochemistry of Carbon Compounds, 2nd Edition, John Wiley & Sons, New York
- 2. D.Nasipuri, 1994, Stereochemistry of Organic Compounds, 2nd Edition, Wiley Eastern Ltd, New Delhi
- 3. PS. Kalsi, 1993, Stereochemistry, Conformation Analysis and Mechanism, 2nd Edition, Wiley Eastern Limited, Chennai

- 4. P.S. Kalsi, 1994, Stereochemistry and Mechanism Through Solved Problems Wiley Eastern Ltd.
- 5. Niel Isaacs, 1987, Physical Organic Chemistry, ELBS Publications
- 6. R.Bruckner, 2002, Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi
- 7. F.A. Carey and R.J. Sundberg, 2001, Advanced Organic Chemistry, Part A and Part-B, 4th Edition, Plenum Press, New York
- 8. J. March, 1992, Advanced Organic Chemistry, 4th Edition, John Wiley & Sons, Singapore.
- 9. T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.
- 10. T.L. Gilchrist, 1992, Heterocyclic Chemistry, 2nd Edition, Longman, Essex, England
- 11. J.A.Joule and K.Mills, 2000, Heterocyclic Chemistry, 4th Edn, Backwell Science Publishers, England.
- 12. L.A. Pacquette, 1978, Principles of Modern Heterocyclic Chemistry, Benjamin Cummings Publishing Co., London.

Websites:-

- 1. http://info.dome.sdsu,./research/guides/science/org chemistryblr.html
- 2. http://www.liv.ac.uk/chemistry/links/reactions.html
- 3. http://orgchem.chem..<u>uconn.edu/namereact/named.html</u>
- 4. <u>www.gcocities.com/</u> chempen softwar4ee/reactions.html

Core Major Theory- II - Inorganic Chemistry - I

Credits -4

Max.Marks-75

Objectives:-

To impart the theories about bonding and structure of various inorganic compounds and few analytical techniques. The basics of reaction Mechanisms in coordination chemistry are also introduced.

Unit I: Bonding in Inorganic compounds

Poly acids: Isopolyacids and heteropolyacids of vanadium, chromium, molybdenum and tungsten.

Inorganic Polymers: Silicates, structure - properties - correlation and applications - molecular sieves, polysulphur - nitrogen compounds and poly - organophosphazenes.

Unit II: Boron compounds and clusters:-

Boron hydrides: Polyhedral boranes, hydroborate ions, carboranes and metallo carboranes. Wade's rules, preparation and reactions of Boron hydrides.

Metal Clusters: Chemistry of low molecularity metal clusters upto trinuclear metal clusters; multiple metal-metal bonds.

Unit III: Theories of coordination:

Inadequacies of VB Theory- Crystal field theory- d-orbital splitting; octahedral, tetrahedral and square planar-LFSE, concept of weak and strong acids, Spectro chemical

series-evidences for metal ligand orbital overlap,Nephlelauxetic effect,MO theory and energy level diagrams, Jahn-Teller distortion, charge transfer spectra

Unit IV: Stability and stereo isomerism of coordination complexes:-

Stability of complexes: thermodynamic stability – stepwise and overall stability constants, their relationships, factors affecting the stability, HSAB approach , chelate effect, importance of chelates. Chelating agents; types of EDTA titrations; direct and back titrations; replacement titrations; masking and demasking reagents.

Macrocyclic ligands; types; schiff bases; crown ethers; cryptands; Stereochemical aspects; Stereoisomerism in inorganic complexes; isomerism arising out of ligand and ligand conformation; chirality and nomenclature of chiral complexes; optical rotatory dispersion and circular dichroism.

Unit-V -Reaction mechanisms and substitution reactions in coordination compounds:-

Electron transfer reactions; outer and inner sphere processes; atoms transfer reaction, complementary and non-complementary reactions. Formation and rearrangement of precursor complexes, binding ligand, successor complexes, Marcus theory.

Substitution Reactions : Substitution in square planar complexes, reactivity of platinum complexes, influence of entering, leaving and other groups, trans-effect, substitution of octahedral complexes of cobalt and chromium, replacement of coordinated water, solvolytic (acids and bases) reactions applications in synthesis (platinum and cobalt complexes only).Rearrangement in 4 and 6 coordinate complexes: reaction at coordinated ligands-template effect.

Text Books:-

- 1. J.E. Huheey, 1993, Inorganic Chemistry Principles, Structure and Reactivity; IV Edition, Harper Collins, NY.
- 2. F.A. Cotton and G. Wilkinson, 1988, Advanced Inorganic Chemistry A Comprehensive Text, V. Edition, John Wiley & Sons.
- 3. K.F. Purcell and J.C. Kot, 1977, Inorganic Chemistry WB Saunders Co., USA.
- 4. M.C. Day and J. Selbin, 1974, Theoretical Inorganic Chemistry, Van Nostrand Co., NY.
- 5. G.S. Manku, 1984, Inorganic Chemistry, TMG Co.,
- 6. D.A. Skoog, 1985, Principles of Instrumental methods of Analysis, III Edition, Saunders College Publication.
- 7. Willard Merrit, Dean and Settle, 1986, Instrumental methods of Analysis, VI Edition CBS Publication.
- 8. A.I. Vogel, 1985, 1976, Text Book of Qualitative Inorganic Analysis, ELBS III Edition, and IV Edition.
- 9. D.A. Skoog D.M. West, 1982, Fundamental of Analytical Chemistry, IV Edition, Holt Reinheart & Winston Publication.

Suggested Reference Books:-

- 1. D.F. Shrivers, P.W. Atkins and C.H. Langfor 1990, Inorganic Chemistry, CH Langford, OUP
- 2. N.N. Greenwood and Earnshaw, 1984, Chemistry of the Elements, Pergamon Press, NY.
- 3. F.A. Kettle, 1973, Coordination Chemistry, ELBS.
- 4. K. Burger, 1973, Coordination Chemistry, Burtterworthy.
- 5. Basolo and R.G. Pearson, 1967, Mechanism of Inorganic Reactions, Wiley, NewYork.
- 6. R.Sarker, general and Inorganic chemistry, (Parts I and II), New Book Agency, Calcutta
- 7. G.D. Christian & J.E.O. Reily, 1986, Instrumental Analysis, II Edition, Allegn Becon.
- 8. H.A. Strobel, 1976, Chemical Instrumentation, Addison Wesley Publ. Co.
- 9. Kolthoff and Elwing (all series), Treatise on Analytical Chemistry.
- 10. Wilson and Wilson series, Comprehensive Analytical Chemistry.
- 11. R.C. Kapoor and B.S. Aggarwal, Ms. 1991, Principles of Polarography, Wiley Eastern Limited.

Core Major Theory - III – Physical Chemistry - I

Credits -4

Max.Marks-75

Objectives:-

To learn the basic concepts in chemical kinetics and group theory and the inadequacy of classical mechanics leading to the formation of quantum mechanics. Mathematical basic for quantum mechanics must be taught.

Unit I: Thermodynamics - I:-

Partial molar properties - Partial molar free energy (Chemical potential) - Partial molar volume and partial molar heat content - their significance and determination of these quantities. Variation of chemical potential with temperature and pressure.

Thermodynamics of real gases - gas mixture - fugacity definition - determination of fugacity variation of fugacity with temperature and pressure -thermodynamics of ideal and non ideal binary solutions-dilute solutions-excess functions for non-'ideal solutions and their determination-the concepts of activity and activity coefficients-determination of standard free energies.

Unit II: Chemical Kinetics - I

Effect of temperature on reaction rates - collision theory - molecular beams - collision cross sections - effectiveness of collisions - probability factors - potential energy surfaces – transition state theory - partition functions and activated complex. Eyring equation - estimation of free energy, enthalpy and entropy of activation and their significance.

Unit III: Chemical Kinetics - II

Reactions in solutions - effect of pressure, dielectric constant, ionic strength and salt effect - kinetic isotopic effects - linear free energy relationships-Hammett and Taft equations - Homogeneous catalysis - Acid base catalysis - mechanisms and Bronsted catalysis law.

Unit IV: Group theory - I

Symmetry elements and operations. Concepts of groups, Sub groups, class, order, Abelian and Non-Abelian point groups. Products of symmetry operations and group multiplication table, point groups-identification and determination-reducible and irreducible representations-Direct product representation-orthogonality theorem and its consequences-character table – construction(NH₃, H₂O).

Unit V: Group theory - II:

Hybrid orbital in non-linear molecules (CH₄, XeF₄, BF₃, SF₆ and NH₃). Determination of representations of vibrational modes in non-linear molecules (H₂O, CH₄, XeF₄, BF₃, SF₆ and NH₃)

Symmetry selection rules for infrared, Raman and electronic Spectra - mutual exclusion principle. Electronic Spectra of Ethylene and formaldehyde-Applications of group theory.

Text Books

- 1. G.K. Vemulapalli, 2000, Physical Chimistry, Prentice Hall.
- 2. J. Rajaram and J.C. Kuriacose, 1993, Kinetics and mechanism of chemical transformations, MacMillan India Ltd.
- 3. K.J. Laidler, 1987, Chemical Kinetics, Harper and Row, New York.
- 4. K. L. Kapoor, 2001, A Text book of Physical Chemistry, Macmillan India Ltd.
- 5. V. Ramakrishnan and M.S. Gopinathan, 1988, Group Theory in Chemistry, Vishal Publications.
- 6. P.W. Atkins, 1990, Physical Chemistry, Oxford.
- 7. K.V. Raman, 1990, Group theory and its applications to Chemistry, Tata McGraw Hill.
- 8. D.A. McQuarrie, 1983, Quantum Chemistry, University Science Books, Mil Valley, California.
- 9. I.N. Levine, 1983, Quantum Chemistry, Allyn and Bacon, Boston.
- 10. R. Anantharaman, 2001, Fundamentals of quantum chemistry, Macmillan India Limited.
- 11. R.K. Prasad, 1992, Quantum Chemistry, New Age, India.

Suggested Reference Books:-

- 1. W.J. Moore, 1972, Physical Chemistry, Orient Longman, London.
- 2. L.K. Nash, 1962, Elements of Chemical Thermodynamics, Addision Wesley.
- 3. G.M. Barrow, 1988, Physical Chemistry, McGraw Hill.
- 4. R.G. Frost and Pearson, 1981, Kinetics and Mechanism, Wiley, New York.
- 5. Moore and R.G. Pearson, 1981, Kinetics and Mechanism.
- 6. I. Amdur and G.G. Hammes, 1968, Chemical Kinetics, Principles and selected topics, McGraw Hill, New York.
- 7. G.M. Harrus, 1966, Chemical Kinetics, D.C. Health and Co.
- 8. F.A. Cotton, 1971, Chemical Application of Group Theory, John Wiley and Sons Inc., NewYork.
- 9. Alan Vincent, 1977, Molecular symmetry and Group theory-programmed introduction to Chemical Aplications, Wiley, New York.

Core Elective-I Polymer Chemistry

Credits -3

Max.Marks-75

Objectives:-

To know about various types of polymers and their properties. Application of the polymer in the present context and its biodegradation is included.

Unit I: Methods of polymerization:-

Basic concepts of polymer chemistry: Repeating unit, degree of polymerisation, classification, stereochemistry of polymers and nomenclature of stereoregular polymers.

Chain, free radical, ionic and ring opening polymerizations. Ziegler – Natta catalyst involment in step polymerisation ring opening polymerisation.

Copolymerisation: Block and graft copolymers – preparation.

Unit II: Properties of polymers:-

Polymerisation techniques: Bulk, solution, suspension and emulsion polymerisation. Melt, solution and interfacial polycondensation. Solid and gas phase polymerisation.

Molecular weight and size: Number and weight average molecular weights. Polydispersity and molecular weight distribution in polymers, the practical significance of polymer molecular weights and size of polymers. (Molecular weight determination is not required)

Glass transition temperature: Concept, associated properties and determination. Glassy solids and glass transition. Factors influencing it.

Crystallinity in polymers: Polymer crystallisation, structural and others factors affecting crystallisability and effect of crystallinity on the properties of polymers.

Unit III: Resins and plastics:-

Processing: Calendering, die casting, rotational casting. Compression, injection, blow and extrusion moulding. Thermoforming, foaming and reinforcing techniques.

Synthetic resins and plastics: Manufacturing and applications of polyethylene, PVC, teflon, polystyrene, polymethylmethacrylate, polyurethane, phenol – formaldehyde resins, urea – formaldehyde and melamine – formaldehyde resins and epoxy polymers.

Unit IV: Synthetic fibers and rubbers:-

Synthetic fibers: Rayon, nylons, polyesters, acrylics, modacrylics and spinning techniques.

Synthetic rubber: SBR, butyl rubber, nitrile rubber, neoprene, silicone rubber and polysulphides.

Conducting polymers and applications.

Unit V: Degradation of polymers:-

Polymer degradation: Types - thermal, mechanical, photo, hydrolytic and oxidative degradations.

Additives for polymers: Fillers, plasticisers, thermal stabilizers, photo stabilizers, antioxidants and colourants.

Biodegradable Polymers and their applications.

REFERENCE BOOKS

- 1. V. R. Gowarikar, N.V. Viswanathan and JayadevSreedhar "Polymer Science" New Age international (P) ltd., Publishers New Delhi, 2005.
- Fred W. Billmeyer, JR "Text book of polymer science" A wiley interscience publication John wiley& sons, New Yark, 1994
- 3. Ayodhya sing "polymer Chemistry" campus Books, New Delhi, 2003

Core Practical -I - Organic Chemistry Practical -I

Credits -4

Max.Marks-60

Objectives:-

To train the students to synthesize an organic compound in single step and to carry out the qualitative analysis of binary organic mixture

I. Analysis of the organic mixture:-

Separation and Identification of components in a two component mixture and preparation of their derivatives.

II. Preparation of the following (Any five)

1	C	. . .	111
1.	Sym-Tribromob	benzene from	aniline.

- 2. p-nitro aniline from acetanilide
- 3. m-Nitrobenzoic acid from methyl benzoate.
- 4. Methyl orange from sulphanilic acid
- 5. m-Nitro benzoic acid from benzaldehyde
- 6. p-bromoaniline from acetanilide
- 7. p-Nitrobenzoic acid from p-Nitrotoluene
- 8. m-Nitroaniline from m-dinitrobenzene
- 9. Anthroquinone from anthracene

III. Quantitative estimation of organic compounds

- 1. Estimation of aniline
- 2. Estimation of phenol
- 3. Estimation of glucose (Bertrands Methods)

Recommended Books:-

- 1. Arthur I. Vogel, A Text Book of Practical Organic Chemistry.
- 2. Raj K. Bansal, Laboratory Manual of Organic Chemistry, Wiley Eastern Limited.
- 3. Mann and Saunders, Laboratory manual of Organic Chemistry

Semester II

Core Major Theory - IV – Organic Chemistry - II

Credits -4

Max.Marks-75

Objectives:-

This paper explains the basic concepts of addition reaction of carbon carbon double bond and elimination reactions. In addition mechanism of some of the important rearrangements in organic chemistry will be discussed. The salient features of oxidation and reduction reactions in organic synthesis are discussed at the end.

Unit I: Addition to carbon-carbon and carbon-hetero multiple bonds

Nucleophilic addition to carbonyls and Stereo Chemical aspects through various model -Crams rule- Prevost rule on addition reaction. Mechanism of electrophilic, nucleophilic and neighbouring group participation in addition reactions. Addition of halogen and nitrosyl chloride to olefins, hydration of olefins and acetylenes, hydroboration, Lithium and boron enolates in aldol, Michael reactions. Alkylation and Acylation using Lithium enolates, hydrogenation of ethylene and acetylene- partial reductions- Homogeneous hydrogenation- Wilkinson's catalyst.

Ylides: Chemistry of phosphorous and sulfur ylides – Wittig and related reaction, Peterson Olification. Diels Alder reaction, 1, 3-dipolar additions, carbenes and carbenoids - addition to double bonds - Simmon Smith reaction, Mannich, Knoevengal, Stobbe condensation, Shapiro reaction, Julia olefination, Acyloin condensations, Darzen, and benzoin reactions.

Unit II: Elimination and Free radical reactions:-

E1, E2 and E1cB mechanism - Orientation of the double bond. Regio selectivity and stereoselectivity of elimination reactions in cyclic systems, pyrolytic eliminations. Chugaev, Hofmann and Cope Elimination.

Long and short lived free radicals - methods of generation. Adddition of free radicals to olefinic double bonds. Sandmayer - Gombereg-Gauchmann, Pschorr, Ulmann and Hunsdicker reactions.

Unit III: Organic Photochemistry and Aromaticity:-

Aromaticity of benzenoid, non-benzenoid and heterocyclic compounds, Huckel's rule-Aromatic systems with pielectrons - numbers other than six non-aromatic (cyclooctatetraene etc) and anti-aromatic systems (cyclobutadiene etc)- with more than 10 pi electrons – Annulenes up to C_{18} (synthesis not expected).

Photo chemistry of ketones, photo oxygenation, photo reduction, photocycloaddition, Paterno - Buchi reaction, Di –pi- methane rearrangement. cis- trans isomerisation, Barton reaction, photo- Fries reaction, photochemistry of cyclohexadienones ,synthesis of Vitamin-D.

Unit IV: Molecular rearrangements:-

A detailed study of the mechanism of the following rearrangements with suitable examples Pinacol-Pinacolone (examples other than tetramethyl ethylene glycol) - Wagner-Meerwein, Demjanov, dienone-phenol, Favorski, Baeyer-Villiger, Cope, Claisen, Stevens, Sommelet-Hauser (in cyclic systems also) and Von Richter rearrangements.

Unit V: Oxidation and reduction reactions:-

Oxidation: Mechanism - study of the following oxidation reactions - oxidation with LTA, SeO₂, DDQ, Oxalyl chloride, Dess-martin reagent DMSO in combination with DCC or acetic anhydride in oxidizing alcohols – Hydroxylations with – OsO₄, KMnO₄, Woodward prevost, epoxidation (per oxides/per acids). Sharpless asymmetry epoxidation,asymmetry dihydroxylations,AD mix,Reduction and Selectrides and Alanes.

Reductions: Synthetic importance of Clemensen and Wolf-Kishner reductions and its

Modifications, Birch reduction, MPV reduction.

Text Books:-

- 1. R.Bruckner, 2002, Advanced Organic Chemistry, Reaction Mechanism, Elsevier, New Delhi
- 2. F. A . Carey and R.J. Sundberg, 2001, Advanced Organic Chemistry, Part A and Part-B, 4th Edition, Plenum Press., New York
- 3. J.March, 2002, Advanced Organic Chemistry, 4th Edition, John Wiley & Sons Singapore.
- 4. T.L. Gilchrist and C.W. Rees, Carbenes, Nitrenes and Arynes, Thomas Nelson and Sons Ltd., London.
- 5. Niel Issacs, 1987, Physical Organic Chemistry, ELBS Publications.
- W. Carruthers, 1993, Some Modern Methods of Organic Synthesis, 3rd Edition, Cambridge University Press.
 Reduction:- Hydride transfer reagents.
 NaBH₄, LiAlH₄, DIBAL-H, Red-Al, Selectrides, Et₃SiH and Bu₃SnH
- 7. H.O. House, 1972, Modern Synthetic Reactions, The Benjamin Cummings Publishing Company, London.

Websites:-

- 1. http://info.dome.sdsu,./research/guides/science/org chemistryblr.html
- 2. http://www.liv.ac.uk/chemistry/links/reactions.html
- 3. http://orgchem.chem..uconn.edu/namereact/named.html
- 4. <u>www.gcocities.com/</u> chempen softwar4ee/reactions.html

Core Major Theory - V – Inorganic Chemistry - II

Credits -4

Max.Marks-75

Objectives:-

The student can gain the knowledge and understanding of all aspects of inorganic polymers, solid state and nuclear chemistry.

Unit I : Solid State Chemistry:-

Preparation Methods: Ceramic method – Sol-gel method – Hydrothermal synthesis – chemical vapour deposition: Structure of Solids: Structure of ZnS, Rutile, Pervoskite, Cadmium iodide and nickel arsenide; spinels and inverse spinels; defects in solids, non-stoichometric compounds - High Temperature Superconductors

Band theory, Semiconductors, Superconductors, Solid State Electrolytes, Types of Magnetic Behaviour - Dia, Para, Ferro, Antiferro and Ferrimagnetism, Hysterisis, Solid State Lasers, Inorganic Phosphorus, Ferrites, Garnets.

Reactions in solid state and phase transitions, diffusion, diffusion coefficient, diffusion mechanisms, vacancy and interstitial diffusion, formation of spinels.

Solid solutions: Order-disorder transformations and super structure.

Unit II: Organometallic Chemistry:-

3.1 Carbon donors: Alkyls and aryls, metalation, bonding in carbonyls and nitrosyls, chain and cyclic donors, olefin, acetylene, and allyl systems. Metallocenes: synthesis, structure and bonding.

3.2 Reactions: Association, substitution, addition, elimination, ligand protonation, electrophilic and nucleophilic attack on ligands, carbonylation, decarboxylation and oxidative addition.

Unit III: Industrial applications of Organo Metallic compounds:-

Catalysis – Hydrogenation of olefins (Wilkinson's catalyst), hydroformylation of olefins using cobalt or rhodium catalyst(Oxo process), oxidation of olefins to aldehydes and ketones(Wacker process):polymerisation(Ziegler-Natta catalyst); Cyclo oligomerisation of acetylene using nickel catalyst(Reppe's catalyst), polymer bound catalysts. Ziegler-Natta catalysis (metallocene and Nom-Metallocene type catalyst).

Unit IV: Inorganic Photochemistry:-

Principles of Inorganic Photochemistry – Photoredox reactions and photosubstitution reactions in coordination complexes with particular reference to Co(III), Cr(III) and Pt(II) complexes. Photosensitisation reactions of [Ru(bpy)3]2+ complex and its applications in solar energy conversions and DSSC's (Dye Sensitized Solar Cells)

Unit V: Nuclear Chemistry:-

Nuclear properties-nuclear spin and moments, origin of nuclear forces. Types of radioactive decay: Orbital electron capture, nuclear isomerism, internal conversion, detection and determination of activity by cloud chamber, nuclear emulsion, bubble chamber, G.M., Scintillation and Cherenkov counters; Accelerators- Linear and Cyclotron Nuclear reaction: Types, reaction cross section, Q-value, threshold energy, compound nucleus theory: high nuclear reactions, nuclear fission and fusion reactions as energy sources; photonuclear and thermo nuclear reactions.

Radioactive tracers: Preparations - principles of tracer technique - application of tracers in the study of reaction mechanism and in analytical chemistry - neutron activation analysis, isotope dilution analysis - radio chemical determination of age of geological specimen. Tracers as applied to industry and agriculture - radioactive tracer in the diagnosis and treatment in the field of medicine.

Text Books:-

- 1. K.F. Purcell and J.C. Kotz, 1977, Inorganic Chemistry WB Saunders Co., U.S.A.
- 2. J.E. Huheey, 1993, Inorganic Chemistry, IV Edition, Harper and Collins, NY.
- 3. F.A. Cotton and G.W. Wilkinson, 1988, Advanced Inorganic Chemistry A Comprehensive Text; John Wiley & Sons.
- 4. B.E. Dogulas DH MX Daniels and Alexander, 1983, Concepts and Models of Inorganic Chemistry, Oxford IBH.
- 5. W.U. Mallik, G.D. Tul, R.D. Madan, 1992, selected topics in Inorganic Chemistry, S. Chand & Co., New Delhi.
- 6. A.R. West, 1991, Basic Solid State Chemistry, John Wiley.
- 7. W.E. Addison, 1961, Structural Principles in Inorganic Chemistry, Longman.
- 8. M. Adams, 1974, Inorganic Solids, John Wiley Sons.
- 9. S. Glasstone, Source Book on Atomic Energy, East West Press.
- 10. C.R. Choppin and J. Ryd Berg: Nuclear Chemistry Theory and Applications, Pergamon Press.
- 11. B.G. Harvey, Introduction to Nuclear Physics and Chemistry Prentice Hall, 1962.

Suggested Reference Books:-

- 1. S.F.A. Kettle, 1973, Coordination Chemistry, ELBS.
- 2. B.N. Figgis, 1966, Introduction to Ligand Fields, Interscience.
- 3. M.N. Hughes, 1982, The Inorganic Chemistry of Biological processes, II Edition, Wiley London
- 4. D. Nicholas, 1974, Complexes of First Row Transition Elements.
- 5. M.C. Shrivers, PW. Atkins, CH Langford, 1990, Inorganic Chemistry, OUR
- 6. M.C. Day and J. Selbin, 1974, Theoretical Inroganic Chemistry, Van Nostrand Co., NY.

- 7. G.S. Manku, 1984, Inorganic Chemistry, TMH.
- 8. U. Sathyanarayana Essentials of Biochemistry, Books and Allied (P) Ltd.
- 9. A.F. Wells, 1984, Structural Inorganic Chemistry, V. Edition, Oxford
- 10. A.R. West, 1990, Solid State Chemistry, John Wiley.
- 11. G.D.Christian & J.E.O. Reily, 1986, Instrumental Analysis, II Edition, Allegn Recon.
- 12. H.A. Strobel, 1976, Chemical Instrumentation, Addition- Wesely Publ. Co.
- 13. Kolthoff and Elwing (All Series) Treatise on Analytical Chemistry.
- 14. Willson Series Comprehensive Analytical Chemistry.
- 15. H.A.O. Hill and P. Day, 1968, Physical methods in Advanced Inorganic Chemistry, JohnWiley.
- 16. K. Burger, 1973, Coordination Chemistry, Experimental methods, Butterworths.
- 17. C.N.R. Rao, J.R. Ferraro, 1970, Spectroscopy in Inorganic Chemistry, Vol. I and Vol. II, Academic Press.
- 18. G. Aruldas, Molecular Structure and Spectroscopy, Prentice Hall.
- 19. E.L. Mutterties, 1975, Polyhedral Borneds, Academic Press, NY.
- 20. NH Ray, 1978, Inorganic Polymers, Academic Press.
- 21. C. Kellter: Radiochemistry, Ellis Hardwood Ltd., John Wiley and Sons.
- 22. G.R. Chopin, Experimental Nuclear Chemistry, Prentice Hall, 1962.
- 23. G. Friedlander, J.W. Kennedy, and J.M. Miller, Nuclear and Radio Chemistry, John Wiley.

Core Major Theory VI – Physical Chemistry - II

Credits -4

Max.Marks-75

Objectives:-

To learn the concepts in enzyme kinetics, surface reactions and fast reactions, and also to understand the formulation and applications of quantum mechanics in atomic and molecular structure. In addition to learn fundamentals of spectroscopy.

Unit I: Thermodynamics - II

Concept of thermodynamic probability - distribution of distinguishable and nondistinguishable particles .Maxwell-Boltzmann, Fermi-Dirac and Bose Einstein statistics modes of contribution to energy- Partition function - translational, vibrational and rotational partition functions for mono, diatomic and polyatomic ideal gases.

Thermodynamic functions in terms of partition functions, Sackur-Tetrode equation equilibrium constant for isotope exchange and dissociation of diatomic molecules;

Unit II: Thermodynamics - III

Heat capacity of solids (Einstein and Debye Models) ortho and para hydrogen -Planck's radiation law - electrons in metals.

Non equilibrium processes ,entropy production in irreversible processes ,microscopic reversibility, linear force and flux relations, Onsager's law, phenomenological equations, Curie's theorem

Unit III: Chemical Kinetics - III

Catalysis by Enzymes-rate of enzyme catalyzed reactions, Michaelis-Menten equation effect of substrate concentration, pH and temperature - inhibitions of enzyme catalyzed reactions – three types with mechanism. Heterogeneous catalysis, Langmuir and BET adsorption isotherms- Kinetics of Heterogeneous catalysis, Unimolecular and Bimolecular reaction. Kinetics and mechanism of surface reactions-catalysis by metals, Hydrogenations and semiconductor oxides. Kinetics of complex reactions – reversible, consecutive and parallel reactions. Chain reactions: general treatment. Rice Herzfeld Mechanism -Decomposition of acetaldehyde and hydrobrominations. Comparison of HCl and HBr formation and explosion limits.

Study of fast reactions-relaxation methods-temperature and pressure jump -stopped flow and flash photolysis methods.

Unit IV: Quantum Chemistry - I

Inadequacy of classical theory - black body radiation, photo electric effect - the Compton effect - Bohr's Quantum theory and subsequent developments -wave particle duality- de Broglie equation, Heisenberg uncertainty principle.

Unit V: Quantum Chemistry - II

Quantum mechanical postulates- Eigen value and function - the Schrodinger wave equation-elementary applications of Schrodinger's equation-the particle in a box (one, two and three dimensional cases) - particle in a ring.
Text Books

- 1. J.Rajaram and J.C.Kuriakose, 1993, Kinetics and mechanism of chemical transformations, Macmillan India Ltd.
- 2. K.J.Laidler, 1987, Chemical Kinetics, Harper and Row, New York.
- 3. D.A. McQuarrie, 1983, Quantum Chemistry, University Science Books, Mil Valley, California.
- 4. I.N. Levine, 1983, Quantum Chemistry, Allyn and Bacon, Boston.
- 5. R. Anantharaman, 2001, Fundamentals of quantum chemistry, Macmillan India Limited.
- 6. R.K. Prasad, 1992, Quantum Chemistry, Wiley Eastern, New Delhi.

Suggested Reference Books:-

- 1. R.G.Frost and Pearson, 1961, Kinetics and Mechanism, Wiley, New York.
- 2. W.J.Moore and R.G.Pearson 1981, Kinetics and Mechanism.
- 3. R.K.Prasad, 1992, Quantum Chemistry, Wiley Eastern, New Delhi.
- 4. J.Goodman, 1997, Contemporary Quantum Chemistry, An Introduction, Plenum Press, New York.
- 5. R.Mcweeny, 1979, Coulon's Valence, ELBS Oxford University Press.
- 6. F.J.Bockhoff, 1976, Elements of Quantum theory, Addison Wesley, Reading Mass.
- 7. P.W.Atkins, 1990, Physical Chemistry, Oxford University Press.
- 8. H.Eyring, J.Walter and G. Gimball, 1944, Quantum Chemistry, John Wiley and Sons, New York.
- 9. L.S.Pauling and F.B.Wilson, 1935, Introduction to Quantum mechanics, Mc Graw Hill Book Company, New York.
- 10. P.W.Atkins, 1983, Molecular Quantum Mechanics, Oxford University Press, Oxford.

Core Elective-II Nano chemistry

Credits -3

Max.Marks-75

UNIT - I

Fundamentals and overview of nanoscience

Nano revolution -Basic idea of nano materials-Structure-Nucleation and grain growth-Grain boundaries-Properties at Nano scale: Strength and Hardness, optical, electrical, magnetic, mechanical and chemical properties.

UNIT - II

Synthesis of nanomaterials

Top down approach – Nanolithography, Chemical Vapour Deposition (CVD). Bottom up approach - sol-gel processing, chemical synthesis. self-assembly- Supramolecular approach. Reverse micelles and role of surfactants- capping of nanoparticles. Synthesis, purification, properties and uses of CNT, metal Nanoparticles. Nano tubes, Nano rods, Bucky balls-fullerenes, Nanofibers, Nanoshells. Semiconductor Nanoparticles- Energy band structure of Semiconductors Quantum dots-Quantization effect.

UNIT - III

Characterisation of nanomaterials- I Theories and Techniques used for characterization-UV-Visible and PL spectroscopy-XRD-Electron microscopes-SEM, TEM, HR-TEM (SAED).

UNIT -IV

Characterisation of nanomaterials- II

Theories and Techniques used for characterization SPM, AFM, STM, XPS, XANES

UNIT - V

Applications of nanomaterials

Solar energy conversion and catalysis - Uses of Nano composites, Nanoelectronics, Liquid crystalline systems, Linear and non-linear optical and electro optical propertiesphotonics, plasmonics, chemical and biosensors. Nanomedicine and Nano biotechnology-NEMS. Nanoparticles in Pollution control. Nano materials in bone substitutes and dentistry, Food and cosmetic applications, textiles, paints, drug delivery and its applicationnanoparticles in cancer targeting and treatment. Nanotechnology in agriculture, fertilizer and pesticides.

REFERENCE BOOKS

- 1. Pradeep, T., "Nano: the Essentials", Tata McGraw Hill, New Delhi, 2007.
- 2. Rao, C.N.R. and Cheetham, A.K., "The chem. of Nanomaterials: Synthesis, Properties and Applications", Wiley-VCH, 2004.
- Hari Singh Nalwa, "Nanostructured materials and Nanotechnology", Acad. press, 2002.Charles P. Poole and Frank J. Owens, "Intro. to Nanotechnology" Wiley-Intersci., 2003.
- 4. A.Nabok, "Organic and Inorganic Nanostructures", Artech House, 2005.
- 5. Sulabha K. Kulkarni, "Nanotech.: Principles and Practices", Capital Publishing Co, 2007.

Core Practical-II Inorganic Chemistry Practical -I

Credits -4

Max.Marks-60

Objectives:-

To train the candidate in preparing inorganic compounds, the detection and identification of **4** cations by semi micro method.

Unit I

Semi micro qualitative analysis of mixtures containing two common and two rare cations. The following rare cation are included: W, Mo, Ti, Te, Se, Ce, Th, Zr, V, U and Li.

Unit-II Colorimetric analysis

Spectrophotometric method: Estimation of iron, nickel, manganese and copper.

Text Books:-

- 1. Vogel, Text book of Inorganic quantitative analysis.
- 2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.

NON MAJOR ELECTIVE-I

Credits -3

Max.Marks-75

Chromatographic Techniques

Objectives:-

This paper enables a student to understand the basic principles of various chromatographic techniques and also instrumentation.

Unit I: Chromatography – General

Chromatographic methods, general aspects of chromatography, Types and mechanism.

Unit II: Column Chromatography (CC)

Column chromatography: construction and operation of column, choice of adsorbents and applications. Ion exchange chromatography: Anion & cation exchangers techniques and applications.

Unit III: Paper Chromatography (PC)

Paper chromatography: Principles, method, recent advancements and applications. Thin layer chromatography: Techniques, choice of adsorbents and applications.

Unit IV: Gas-liquid Chromatography (GLC)

Gas-liquid Chromatography: Principles, Retention Volumes, Instrumentation, Carrier Gas, Columns, Stationary Phase, Detectors, Thermal Conductivity, Flame Ionization, Electron Capture and applications.

Unit V: High Performance Liquid Chromatography (HPLC)

High Performance Liquid chromatography: scope, column efficiency, instrumentation, pumping systems, column packing, detectors and applications.

Text Books:-

- Vogel's, 2000, Text book of Quatitative Chemical Analysis, Sixth Edition, Pearson Education Limited, London.
- D. A. Skoog and J. J.Leary, 1971, Principles of Instrumental Analysis, Fourth Edition, Saunders College Publishing, US.

Semester III

Core Major Theory-VII – Organic Chemistry – III

Credits -4

Max.Marks-75

Objectives:-

The first part of the paper explains the instrumental methods and their application in the determination of structure of organic molecules. The second part includes the basic concepts of aromaticity and photochemistry. A detailed account of orbital symmetry which forms the basis of many organic reactions is also included. The last part of the subject deals with heterocyclics, terpenoids and steroids.

UNIT - I IR AND RAMAN SPECTROSCOPY

IR Spectroscopy : Skeletal vibrations and finger print regions – characteristic vibrational frequencies of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols and amines, carbonyl compounds (ketones, aldehydes, esters, amides, acids, anhydrides, lactones, lactams and conjugated carbonyl compounds) - Effect of Hydrogen bonding and solvent effect on vibrational frequencies – extension to various organic molecules for structural assignment

Raman Spectroscopy: Application in organic chemistry – Benzene: ortho, para, meta isomers- cis, trans isomers – structure determination by combined use of Raman and IR spectra

UNIT - II UV SPECTROSCOPY

Types of transitions – Woodward Fieser rules – differentiation of geometrical isomers and position isomers (disubstituted benzene derivatives, nitrophenols) conjugated cyclic ketones, acetophenones, esters – study of steric effect in aromatic compounds – steric inhibition of resonance.Solvent effects.

UNIT - III

¹H NMR SPECTROSCOPY

Nuclear Magnetic Resonance Spectroscopy: Approximate chemical shift values of various chemically non-equivalent protons and correlation to protons bonded to carbon (aliphatic, olefinic, aldehydic and aromatic), Protons bonded to other nuclei (alcohols, phenols, enols, carboxylic acids, amines, amides, SH), Chemical exchange, effect of deuteration, complex spin-spin interaction between two, three, and four interacting nuclei (first order spectra), Complex interaction, virtual coupling, stereochemically hindered rotation, Karplus curve, variation of coupling constant with dihedral angle, nuclear magnetic double resonance, simplification of complex spectra using shift reagents and Nuclear Overhauser Effect (NOE). Solid state NMR, MAS,NMR applications, NMR of some Polymers.

Unit - IV

¹³C NMR SPECTROSCOPY

¹³C NMR Spectroscopy: Chemical shift (aliphatic, olefinic, alkynes, aromatic, heteroaromatic, carbonyl carbon), Coupling constants. Applications of IR, NMR, and Mass spectroscopy for structure elucidation of organic compounds.

UNIT - V

MASS SPECTROMETRY

Mass spectral fragmentation of organic compounds – common functional groups – molecular ion peaks – meta stable peak – McLafferty rearrangement – general rules for

interpretation of the spectrum – molecular weight, isotope effect, nitrogen rule, ring rule – examples of mass spectral fragmentation of organic compounds with respect to their structure determination – applications – molecular weight determination, isotopic abundance, bonding information, determination of bond dissociation energies, impurity detection, identification of unknown compounds, characterization of polymers.

REFERENCE BOOKS

- R. M. Silverstein, F. X. Webster, and D. Kiemle, Spectroscopic Identification of Organic Compounds, 7th Ed., John Wiley & Sons, 2005.
- R. S. Macomber, A complete introd. to modern nmr spectroscopy, John Wiley & Sons, 1998.
- 3. E. D. Becker, High resolution NMR, 3rd Ed., Academic Press, 1999.
- 4. D. L. Pavia et al., Introduction of spectroscopy, 4th Ed., Brooks Cole, 2008.
- 5. W. Kemp, Organic Spectroscopy, 3rd Ed., McMillan Press Ltd., 1991.
- D. H. Williams & I. Fleming, Spectroscopic Methods in Organic Chemistry, 5th Ed., Tata McGraw Hill, 2004.
- C. N. Banwell& E. M. McCash, Fundamentals of Molecular Spectroscopy, Tata Mc-Graw-Hill, New Delhi, 2006.
- D. Pasto, C.Johnson&M.Miller, Experiments and Techniques in Organic Chemistry, Prentice Hall Inc., New Jersey, 1992
- 9. Barrow, Molecular Spectroscopy, McGraw Hill Book Co., 1962.
- D. N. Sathyanarayana, Vibrational spectroscopy Theory and Applications, Ist Ed., New Age International Ltd., New Delhi.

Text Books:-

- 1. R.M. Silverstein, G.C. Bassler and Morril, 1991, Spectrometric identification of Organic Compounds, 5th Edition, John Wiley and Sons, New York.
- 2. I.L. Finar, 1986, Organic Chemistry Vol.II, 5th edition, ELBS Publication.
- 3. P.S. Kalsi, 2002, Spectroscopy of Organic Compounds, Wiley Eastern Ltd, Chennai.
- 4. H. Depuy and Orville, Molecular reaction and Photochemistry Charles, L.Chapman, Prentice Hall of India Pvt. Ltd., New Delhi
- 5 J. March, 1992, Advanced Organic Chemistry, 4th Edition, Singapore

- 6 F.A. Carey and R.J. Sundberg, 1990, Advanced Organic Chemistry, 4th Edition, Plenum Press, New York.
- 7 Neil S. Issacs, 1987, Physical Organic Chemistry, ELBS Publication.
- 8. P.S. Kalsi, 1999, Texbook of Organic Chemistry, Mcmillan India Ltd.

Websites:-

- 1. http://info.dome.sdsu, /research/guides/science/org chemistryblr.html
- 2. http://www.liv.ac.uk/chemistry/links/reactions.html
- 3. http://orgchem.chem..uconn.edu/namereact/named.html
- 4. <u>www.gcocities.com/</u> chempen softwar4ee/reactions.html

Core Major Theory – VIII – Inorganic Chemistry – III

Credits -4

Max.Marks-75

Objectives:-

To understand the applications of different spectroscopic methods in the study of Inorganic compounds.

Unit I: IR and Raman Spectra Application:

Effect of coordination on ligand bands- Ammine, Nitro, nitrito, thiocyanato.

Urea complexes, dithiocarbamato complexes, carboxylate complexes, nitrosyl complexes, cyano complexes- nitrate, sulphate and perchlorate complexes- differentiation of geometric isomers. Metal carbonyls, olefin complexes, sandwich complexes.

Raman spectroscopy of metal complexes, organometallic and simple inorganic compounds with special reference to coordination sites, isomerism.

Unit II: Electronic Spectra application:

Classification of Transitions – Selection Rules – Free ion terms – Racah Parameter – Ligand field perturbations on the free ion terms – Spectra of Octahedral complexes: d^n configurations- Weak field and strong field ligands – Orgel and Tanabe-Sugano Diagrams – Evaluation of $10D_q$ – Spectra of distorted octahedral complexes – Jahn-Teller Distorion – Tetrahedral Complexes - Nephelauxetic effect – Charge Transfer Spectra.

Unit III: NMR, NQR and Mossbauer

NMR, NQR, Mossbauer spectra: NMR spectra of ³¹P, ¹⁹F, NMR shift reagents, NQR-Nitrosyl compounds. Mossbauer of Fe and Sn systems.

Unit IV: Application of ESR and Photo electron spectroscopy to coordination

complexes

ESR introduction-Zeeman equation, g value, nuclear hyperfine splitting, Interpretation of ESR spectrum of simple carbon centered free radicals. Anisotropy in g value and hyperfine splitting constant. McConnels equation, Kramer's theorem, esr of transition metal complex of copper, manganese and vanadyl complexes.

Photoelectron spectroscopy – UPS and XPS-Photoelectron spectra – Koopman's theorem,-Fine structure in PES, Chemical shift and Correlation with electronic charges.

Unit V: X-ray diffraction and Microscopy application

Basic Principles of diffraction – Bravis Lattices- Use of X-ray power diffraction data in identifying inorganic crystalline solids. Single crystal diffraction in crystal structure analysis. Optical Microscopy, Electron Microscopy – SEM and TEM. X-ray Flourescence Spectroscopy – structure determination.

Text Books:-

- 1. L.Smart, E.Moore Solid State Chemistry An Introduction-2nd Edition
- 2. A.R.West Basic Solid state Chemistry 1961 John Wiley
- 3. A.R.West Solid state Chemistry and its applications 2007 John Wiley

- 4. W.E Addison, 1961, Structural principles in Inorganic Chemistry, Longman
- 5. Structural principles in inorganic Chemistry –Adams
- 6. Physical methods in inorganic Chemistry Russel Drago
- 7. Physical methods in inorganic Chemistry E.A.V Ebsworth, Rankin and Caddock. 1987.
- 8. Vibrational Spectroscopy Theory and Applications New Age, D.N.Sathyanarayana, 2011.
- 9. Magenetic Resonance Spectroscopy-ESR, NMR, NQR-IK International D.N. Sathyanarayana, 2014.

References:-

- 1. R.B.Heslop and K.Jones, inorganic Chemistry, Elsevier Scintific Publ .1976.
- 2. H.A.O Hill and P.Day, physical methods in dvanced Inorganic Chemistry, John wiley 1968.
- 3. C.N.R Rao, J.R.Ferraro, Spectrosopy in inorganic chemistry, Vol.I and Vol II, Academic press, 1970.
- 4. G.Aruldhas, molecular structures and spectroscopy-Prentice hall.
- 5. M.F.Lappert –Physical inorganic Chemistry-inorganic Electron Spectrosopy 1968.

Core Major Theory- IX - Physical Chemistry – III

Credits -4

Max.Marks-75

Objectives :-

To understand and appreciate the significance and applications of classical thermodynamics, electrochemistry in solutions and to learn the principle and applications of optical and resonance spectroscopy.

Choice of standard states - determination of activity and activity coefficients for nonelectrolytes.

Unit I: Spectroscopy I

Electromagnetic radiation: Quantization of energy- rotational, vibrational and electronic energy levels and transitions in molecules- regions and representation of spectra. Resolution and intensity of spectral transition: signal to noise ratio- width of spectral lines- collision broadening – Doppler broadening – Heisenberg uncertainty principle – intensity of spectral lines- selection rules and transition probability- transition moment integral- Einstein absorption coefficient.

Electronic spectra of polyatomic molecules, Franck-condon principle- selection rules – types of transition in saturated and unsaturated hydrocarbons, effect of conjugation and solvent effects.

Unit II : Spectroscopy - II

Rotational spectroscopy of a rigid rotar – non-rigid rotor-diatomic and polyatomic molecules. Vibrational spectroscopy-harmonic oscillator-anhormonicity –Vibration – rotation spectra of diatomic vibrating molecules selection rules-P,Q and R branches.

Vibrational spectra of polyatomic molecules- fundamental vibrations – normal modes of vibration- overtones, combination and difference bands- Fermi resonance. Raman spectra: Classical theory of Raman effect and molecular polarisability – pure rotational Raman spectra – Vibrational Raman spectra – Rotational fine structure – Rule of mutual exclusion – Polarization of light and Raman effect.

Unit III: Spectroscopy - III

Resonance spectroscopy-Zeeman effect-equation of motion of spin in magnetic fields. AX and AMX type molecules- H¹, ¹³C, ¹⁹F, ³¹P NMR spectra - a brief qualitative discussion of Fourier transform spectroscopy. ESR: principle, spin-orbit coupling. Hyperfine interaction. McConnell reactions.

Mass spectra: Theory and instrumentation, Mossbauer spectroscopy- Doppler effects, isomer shift, electron-neutron hyperfine interactions. Quadrupole interactions and Magnetic interactions.

Unit IV: Quantum Chemistry - III

The harmonic oscillator- the rigid rotor- the hydrogen atom- the Schrodinger equation for hydrogen atom- angular momentum - term symbols -the solution- the origin of quantum numbers (angular momentum and spin) -their physical significance.

Unit V: Quantum Chemistry – IV

Approximation methods –perturbation and variation method –application to hydrogen ,helium atoms –R.S. coupling and term symbols for atoms in the ground state – Slater orbital and HF –SCF methods Born – Heimer approximation –valence bond theory for hydrogen molecule –LACO –MO theory for di and polyatomic molecules –concept of hybridization – Huckel theory for conjugated molecules (ethylene , butadiene and benzene)- semi empirical methods .

Text Books:-

- 1. S. Glasstone, 1960, Thermodynamics for chemists, Affiliated East West Press, New Delhi.
- 2. J. Rajaram and J.C. Kuriacose, 1986, Thermodynamics for students of chemistry, Lal Nagin Chand, New Delhi.
- 3. A. Caringtion and A.D Mc Lachlan, 1967, Introduction to Magnetic Resonance Harper and Row, New York.
- 4. G. Aruldas, 2002, Molecular structure and spectroscopy, Prentice Hall.
- 5. C.N. Banwell, 2003, Fundamentals of Molecular, Spectroscopy Tata McGraw Hill.
- 6. D.N. Sathyanarayana vibrational spectroscopy
- 7. D.N. Sathyanarayana electronic spectroscopy
- 8. J.O.M. Bokris and A.K.N. Reddy, 1977, Electrochemistry, VoIs1 and 2 Plenum, New York..
- 9. J. Robbins -1993, Ions in Solution-An Introduction in electrochemistry, Clarendon press, Oxford
- 10. R.K.Prasad, 1992, Quantum Chemistry, Wiley Eastern, New Delhi.
- 11. D.A. Mcquarrie, 1983, Quantum Chemistry, University Science Books, Mill Valley, Calfornia.

Suggested Reference Books:-

- 1. R.L. De Koch and H.B. Gray, Chemical Structure and Bonding, Benjamin/Cumming, Menlo Park, California.
- 2. J.N. Murrell, S.F.A. Kettle and J.M. Tedder, 1985, The Chemical Bond, Wiley.
- 3. P.W. Atkins, 1983, Molecular Quantum Mechanics, Oxford University Press, Oxford.
- 4. P.H. Rieger, 1994, Electrochemistry, Chapman and Hall, New York.
- 5. W. Kemp, 1986, NMR in Chemistry McMilan Ltd.
- 6. G.W. King, 1964, Spectroscopy and Molecular Structure, Holt Rieneheart and Winston.
- 7. K.D. Mclauchlan, 1970, Magnetic Resonance, Oxford chemistry Series, Oxford.
- 8. B.P.Staughan and S.Walker, 1976, Spectroscopy Vol. 1, 11 and 111, Chapman and Hall.
- 9. B.W. Cook and K. Jones, 1972, A.Programmed Introduction to Infra red spectroscope, Heydon and Son Ltd.
- 10. F.A. Rushworth and D.P Tunstal, 1973, Nuclear Magnetic Rewsonance Gorden and Breaqch Science Publishing, New York.
- 11. J.K. Sanders and B.K.Hunther, 1987, Mordern NMR Spectroscopy, A Guide for Chemists, Oxford University Press, Oxford.
- 12. J.K.M. Sanders, E.C. Constable and B.K. Huntherm Morden, 1989, NMR Spectroscopy - A World Book of chemical problems, Oxford.

Core Elective –III Electrochemistry

Credits -3

Max.Marks-75

UNIT – I

Ionic phenemenona in solution- I

The Born model of ion-solvent interaction. The concept of ionic atmosphere. Debye Huckel equations for the mean activity coefficient of electrolytes- verification and experimental validity of the equation. Bjerrum ion pair theory – Bjerrum modification of Debye Hukel equation.

$\mathbf{UNIT} - \mathbf{II}$

Ionic phenemenona in solution- II

Ion association treatment – diffusion – Fick's law of diffusion – Einstein Smolunchowki equation – conduction – Stoke Einstein equation – transport number of ions – Onsager phenomenological equation – Plank Henderson equation – influence of ionic atmosphere on conductivity of electrolytes. Debye Huckel Onsager equation for the equivalent conductivity of electrolyte – Experimental verification.

UNIT – III

Structure and theories of Electrified Interface

The electrode electrolyte interface – electrical double layer – electro capillary phenomena – parallel plate condenser model – Guoy Chapman diffuse model – Stern model.

Significance of equilibrium exchange, current density and symmetry factor. Butler-Volmer equation for one electron transfer. Electro kinetic phenomena – membrane potential. – Tisselius method of seperation of proteins – Butler Volmer equation for one electron transfer. Significance of equilibrium exchange current density and symmetry factor.

UNIT - IV

Electrochemical systems of technological interest

Corrosion and the stability of metals. Theories of corrosion – charge transfer reaction of corrosion, short circulated energy producing cell, corrosion of ultrapure metals – corrosion current & corrosion potential. Evans diagrams – potential – pH diagram (Pourbaix diagram) – Prevention of corrosion – electronic approach to the stability of metals.

$\mathbf{UNIT} - \mathbf{V}$

Electrode, SHE, dropping calomel electrode, Quinhydrone electrode, glass electrode – merits and demerits. Fuel cells – kinds of fuel cells and their relative merits – electricity storage – Lead storage battery – Lechlanche cell – silver – zinc cell and sodium-sulphur cell.

Reference books

 J. O. M.Bockris and A. K. N. Reddy, Modern Electrochemistry, vol.1 & 2, Plenum Press,

New York, 1970.

- S. Glasstone, Electrochemistry, Affiliated East-West Press Pvt. Ltd., New Delhi, 1974..
- 3. L. Andropov, Theoretical Electrochemistry, Mir Publications, Moscow, 1977.
- 4. J. Rajaram and J. C. Kuriakose, Kinetics and Mechanism of Electrochemical Transformations, Macmillan India Ltd., New Delhi, 1993.

Non Major Elective- II

Credits -3

Max.Marks-75

Environmental Chemistry

Objectives:-

To know the importance of Environment and methods to save our earth from pollution. To learn more about our earth and environment and how to protect our environment.

Unit I: Environment

Introduction, composition of atmosphere, vertical temperature, heat budget of the earth atmospheric system, vertical stability atmosphere, biogeochemical cycles of C, N, P, S and O and biodistribution of elements.

Unit II: Hydrosphere

Chemical composition of water bodies – lakes, streams, rivers and wet lands etc., and hydrological cycle.

Aquatic pollution – inorganic, organic, pesticide, agricultural, industrial, sewage, detergents and oil pollutants. Water quality parameters – dissolved oxygen, biochemical oxygen demand, solids, metals, content of chlorides, sulphate, phosphate, nitrate and micro-organisms. Water quality standards.

Unit III: Solids and Atmosphere

Soils - composition, micro and macro nutrients. Pollution – fertilizers, pesticides, plastic and metals. Waste treatment.

Atmosphere – chemical composition of atmosphere – particles, ions, radicals and their formation.

Chemical and photochemical reactions in atmosphere: smog formation, oxides of N, C, S and O and their effects. Pollution by chemicals, petroleum, minerals, chlorofluorohydrocarbons, green house effect, acid rain, air pollution control and dye chemistry.

Noise pollution.

Unit IV: Industrial pollution

Cement, sugar, distillery, paper and pulp, thermal power plants, nuclear power plants, metallurgy, polymers and drugs etc. Radionucleide analysis. Disposal of waste and their management.

Unit V: Environmental toxicology

Chemical remedy to environmental problems, biodegradability, principles of decomposition, Better industrial processes, Bhopal gas tragedy, Chernobyl, three mile island, Sewozo and Minamata disasters. Toxicity of metals – Cd, Hg, Cr, Cu and Pb.

Recommended Books:

- 1. Environmental chemistry S.E. Manahan, Lewis Publishers.
- 2. Environmental chemistry Sharma and Kaur, Krishna Publishers.
- 3. Environmental chemistry A.K. De, Wiley Eastern Publishers.
- 4. Environmental pollution analysis S.M. Khopkar, Wiley Eastern Publishers.
- 5. Environmental toxicology ED. J. Rose, Gordon and Breach Science Publications.
- 6. Standard methods of chemical analysis F.J. Welcher Vol. III, Van Nostrand Reinhold Co.
- 7. Elemental analysis of air borne particles Ed. S. Landsberger and M. Greatchman, Gordon and Breach Science Publications.
- 8. Environmental chemistry C. Baird, W.H. Freeman.
- 9. Chemistry of our environment R.A. Home.

Core practical-III - Inorganic Chemistry Practical II

Credits -4

Max.Marks-75

Objectives:-

To acquire skill in preparation of coordination complexes and to estimate gravimetrically and volumetrically the given metals ions (Mg, Ni, Zn, Fe and Cu) in the given mixture and analysis of ores and alloys.

Unit I: Preparation of the following:-

- 1. Sodium bis(thiosulphato)cuprate (I)
- 2. Sodium hexanitrocobaltate (III)
- 3. Hexaminenickel (II) chloride
- 4. Bis (thiocynato) pyridine manganese, (II)
- 5. Tris (thiourea) copper (I) chloride
- 6. Potassium tris (oxalato) chromate (III) trihydrate
- 7...Tris (thiourea) copper (I) sulphate

Unit II: Quantitative analysis: Mixture of metal ions (gravimetrically and volumetrically)

- 1 Magnesium and Iron in the mixture of Iron and magnesium
- 2 Nickel and copper in the mixture of copper and nickel
- 3 Zinc and copper in the mixture of copper and zinc.
- 4 Nickel and Iron in the mixture of iron and Nickel.

Text Books:-

- 1. Vogel, Text book of Inorganic quantitative analysis.
- 2. Dougles A. Skoog, Principles of Instrumental Analysis, 3rd Edition.

Semester IV

Core Paper Theory- X– Organic Chemistry – IV

Credits -4

Max.Marks-75

Objectives

This paper introduces the basic methodologies for the synthesis of organic compounds.

Unit I: Pericyclic Reactons

Pericyclic reactions-classification, electrocyclic, cycloaddition reactions. Woodword Hoffman rules, FMO-Analysis of electrocyclic, cycloaddition and sigmatropic reactions-correlation diagram for cycloaddition reaction, butadiene – cyclobutene system and Inter conversion of hexatriene to cyclohexadiene.

Unit II: Alkaloids and Proteins

Structural elucidation and total synthesis of morphine.

Peptides and their synthesis (Synthesis of tripeptide using amino acids - Glycine, Alanine, Lysine, Cysteine, Glutamic acid, Arginine).Merrified synthesis, Determination of primary, secondary and tertiary structure of proteins.

Unit III: Modern synthetic methodology

Application of synthetic methodology for the synthesis of simple cyclic and acyclic target molecules -synthesis of cubane, 5 - hexenoicacid , bicyclo (4, 1, 0) heptane-2-one.,trans 9-methyl-1- decalone ,longifolene and onocerin. Concept of Synthones, synthetic equivalents and intermediates. Formation of C-C and C=C bonds. Reversal carbonyl polarity – Umpolung addition.

Unit IV: Retrosynthetic analysis, Protection and Deprotection

Retro synthetic analysis and synthesis of simple organic molecules such as 1,2, 1,3, 1,4 and 1,5 dicarbonyl compounds both acylic and cyclic. Formation of 3, 4, 5 and 6 membered cyclic compounds - Baldwin's rules. Use of standard reactions, like Grignard reactions, Robinson annulations. Protection and deprotection of functional groups (R-OH, RCHO, R-CO-R, R-NH₂ and R-COOH). Use of PTC (Phase-transfer catalyst) and Crown ethers in organic synthesis.

Unit V: Novel reagents in organic synthesis:-

Synthesis and applications of Organolithium, Organomagnesium, Organozinc and Organo Copper and Gilman reagents. Modern synthetic methods: metal mediated C-C coupling reactions: Mechanism and synthetic applications of Heck, Stille, Suznki, Negishi, Sonogashira, McMurray, Metathesis and Carbonylation reactions. Green reactions and reagents.

Text Books:-

- 1. R.K. Mackie and D.M. Smith. 1998, Guide book to organic synthesis, ELBS Publication.
- 2. I. L. Finar, 1986, Organic Chemistry, 5th Edition, Vol .II, ELBS Publication.
- 3. L. Smith, Robert L. Hill .1. Robert Lehman, Robert J .Iet Rowitz, Philp Handler and abrahim white principles of Biochemistry General aspects, 7th Edition, McGraw Hill Int.
- 4. L. Stryer, Biochemistry, W.H.Freeman and Co., New York.
- 5. Agarwal, Chemistry of Organic Natural Products, Goel Publishing House.
- 6. B.l. Smith, 1980, Organic synthesis, Chapman and Hall, NY.
- 7. Francis.A. Carey, Richard J. Sundbreg, 2001, Advanced Organic Chemistry, 4th Edition, Plenum Press, New York.
- 8. N.J. Turro, 1978 Modern Molecular Photochemistry, Benjamin, Cummings, California.

Websites

- 1. <u>http://infodome.sdsu,./research/guides!science!orgchemistryblr</u>. html
- 2. <u>http://www.liv.ac.uklchemistry/links/reactions.html</u>
- 3. <u>http://orgchem.chem.uconn.edu/namereacVnamed.html</u>
- 4. <u>www.gcocities.com/chempensoftwar4ee/reactions.html</u>)

Core Elective-IV Research Methodology

Credits -3

Max.Marks-75

Objectives:-

The aim is to explain various aspects of research methodology- Literature, planning, data analysis and report writing.

UNIT I: Research Problem

Objectives of research, types of research – basic, applied, and other types.

Problem selection – project proposal - funding agencies.

UNIT II: Source of Literature

Chemistry literature survey –primary, secondary and tertiary sources.

Journals published by the ACS and RSC - CA and its importance -Indian Journals -

reviews, monographs, data books and indexes. Methods of searching, compilation,

preservation and retrieval of collected literature .Impact factor and citation index.

UNIT III: Research planning, methods and materials

Planning and conducting experiments.

Methods of collecting data – primary and secondary –sources of secondary data.

Classification and tabulation of data – types of classification –general rules for tabulation–types of tables.

Simple sampling techniques and size of the sample.

UNIT IV: Analysis of data

Presentation of data - Types of errors – Gross, systematic and random errors.

Measures of central tendency, mean, standard deviation and measures of variability.

Linear regression, correlation and method of least squares.

UNIT V: Report writing

Project report writing – general, chapter and page format.

Procedure for presenting tables, graphs and figures, foot-notes, bibliography and appendices.

Abbreviations, symbols and SI units.

Plagiarism, copy right and patent laws.

Publication of research paper.

Suggested Reference Books:-

Thesis and Assignment Writing – J Anderson, B.H. Dursten and M. Poole, Wiley Eastern (1977).

Statistical Method, Gupta S. P, Sultan Chand and Sons, New Delhi, 2004

Hand Book for Authors –Journal of the American Chemical Society Publications

Chemical publications - Their nature and uses

Core Elective-V-Analytical Techniques in Chemistry

Credits -3

Max.Marks-75

Objectives

The course aims to explain various analytical techniques useful for chemistry. Colorimetric analysis and spectral techniques such as UV-Vis, IR, NMR, NQR, EST, TGA, MS, X-ray and Photoelectrons spectroscopy are objective of students learning.

Unit I: Colorimetric analysis, UV-Vis, IR and Raman spectrum:-

Colorimetric analysis and UV-Visible spectroscopy: Beer Lambert's law, Principles of single and double beam instruments – applications for analysis of inorganic and organic samples.

Infrared spectrophotometric analysis – principle, instrumentation and structure determination.

Raman Spectra – principle, basic instrumentation and structural analysis.

Unit II: NMR and NQR:-

Nuclear Magnetic Resonance – Principle, instrumentation, structure determination. NMR of ¹H, ¹³C, ³¹P, ¹⁹F.

NQR - Nitrosyl compounds, Mossbauer of Fe and Sn systems.

Unit III: ESR and Magnetic properties:-

Electron Spin Resonance – Principle, instrumentation, applications to coordination compounds.

Magnetic Susceptibility and measurements- Guoy method, Faraday method-applications.

Unit IV: TGA, DTA and Mass Analysis

Thermo gravimetric and differential thermal analysis, thermometric titrations, differential scanning colorimetry – basic instrumentation and applications.

Mass Spectrometry- Principle, basic instrumentation, fragmentation patterns structural determination of organic molecules.

Unit V: Atomic absorption spectroscopy and Photoelectron spectroscopy:-

Atomic absorption spectroscopy: Theory, atomizers, flame and electro thermal.

radiation sources, instrumentation, spectral and chemical interferences and application.

Photoelectron spectroscopy (UV and X-Ray)-photo electron spectra-Koopman's

theorem, fine structure in PES, chemical shift and correlation with electronic charges.

Text Books:-

- 1. D.A .Skoog, 1985, Principles of Instrumental Methods of analysis, III Edition, Saunders College Publ.
- 2. Willard Merrit, Dean and Settle, 1986, Instrumental methods of analysis, VI Edition, CBS Publ.
- 3. A.I. Vogel, 1976, Textbook of Qualitative Inorganic Analysis, III Edition, ELBS.
- 4. D.A. Skoog and D.M. West, 1982, Fundamentals of Analytical Chemistry, IV Edition, old Reinhord & Winston, Publication.

Suggested Reference Books:-

- 1. G.D.Christian & J.E.O. Reily, 1986, Instrumental Analysis, II Edition, Allegn Recon.
- 2. H.A. Strobel, 1976, Chemical Instrumentation, Addition- Wesely Publ Co.

- 3. Kolthoff and Elwing (All Series) Treatise on Analytical Chemistry.
- 4. Willson Series Comprehensive Analytical Chemistry.
- 5. H.A.O. Hill and P. Day, 1968, Physical methods in Advanced Inorganic Chemistry, JohnWiley.
- 6. K. Burger, 1973, Coordination Chemistry, Experimental methods, Butterworths.
- 7. C.N.R. Rao, J.R. Ferraro, 1970, Spectroscopy in Inorganic Chemistry, Vol. I and Vol. II, Academic Press.
- 8. G. Aruldas, Molecular Structure and Spectroscopy, Prentice Hall.

Core Practical-IV - Physical Chemistry Practicals

Credits -4

Max.Marks-75

Objectives:-

To understand and verify the principles and theory of physical chemistry experiments. To carry out conductometric and potentiometric experiments in order to acquire skill in the determination of equivalent conductance and solubility product etc.

- Construction of phase diagram for a simple binary system; naphthalene biphenyl, naphthalene –p-dichlorobenzene, naphthalene-diphenylamine.
- Determination of partition coefficient, equilibrium constant and unknown concentration of potassium iodide of the reaction between iodine and potassium iodide by partition method.
- 3. Kinetic study of the reaction between acetone and iodine in acidic medium and determination of the order with respect to iodine and acetone
- 4. Comparison of acid strengths for hydrolysis of methy lacetate catalyzed by acids
- 5. Determination of the rate constant and order for the reaction between potassium persulphate and potassium iodide
- Conductometric titrations of single and mixture of strong and weak acids against strong base.

7. Potentiometric Experiments

- 1. Determination of pH and pKa
- 2. Determination of solubility product of a sparingly soluble salt.
- 3. Potentiometric titrations
 - a. single and mixture of strong and weak acids and strong base
 - b. Redox titrations by emf measurements.
 - c. Precipitation titration of mixture of halides.