M.Sc. Chemistry

(Master of Science – Chemistry)

Jain Global Campus, Jain University

Jakkasandra (P), Kanakapura (T)

Bangalore Rural

Regulations, Scheme of Study and Syllabi

Effective from the academic year 2012-13

M.Sc. Chemistry

(Master of Science – Chemistry)

REGULATIONS

Introduction to the course

The M.Sc Chemistry course is designed to give you an insight into the amazing world of chemical science. Its deals with the study of inorganic, organic, physical, analytical, biochemical, environmental and nanochemistry. The course provides the depth exposure into its application, hands-on training in the various techniques including synthesis and analysis.

1. Scope and content:

1.1 The regulation and policies documented here are applicable for M.Sc. Chemistry programme offered by Jain university.

1.2 The applicability of the regulations and policies must be understood in the context of the given course matrix and syllabus of each programme.

1.3 The regulations and policies given here are in addition to the rules and regulations notified at the time of admission.

1.4 The authorities of university may modify, and delete, expand or substantiate any part of the regulations and policies, at any time.

2. Course content:

The programme shall be for a duration of four semesters, spread out in two years. Each semester of the programme shall consist of the following components:

1. Core subjects
2. Practical subjects
3. Project work

2.1 Core subjects:

Core subjects comprise of subjects that form an integral part of the programme. These subjects provide a strong ground in basic disciplines of study.

2.2 Practical subjects:

These subjects are totally practical-Based subjects. The learning of these subjects will be mainly in laboratories and some cases to practical sites with equipments/resources. These subjects shall support the practical implementation

of the core subjects. The process of evaluation of these subjects will depend on the nature of that individual subject.

2.3 Project Work:

The project work shall be done for duration as specified by the coordinator, in the area, related to the main subject of study or the specialization. The project work shall give the student an insight to the conditions existing in the field of synthesis, characterization, application of materials.

3. Eligibility for admission and mode of selection:

3.1 The minimum qualification required to be eligible for admission is a degree from recognized university with a minimum of 50% marks in aggregate or in the relative /respective subject.

3.2 The method of selection for the course shall normally be by means of a personal interview. However, for some programme, the admission might also be by means of an entrance test.

4. Attendance requirement:

4.1 A student should have attended a minimum of 85% of the classes conducted in each subject. In case student fails to fulfill the 85% attendance requirement, then the Dean/Principal/Head of the department can consider condonation to a maximum extent of 10% provided the candidate has a minimum of 75% attendance in that semester. In exceptional cases, the vice-chancellor may grant 15% condonation. In such cases, the attendance should be more than 70%.

4.2 In case the candidate's attendance falls below 75% in a subject he/she may be permitted to register for the summer term with permission of the board but no candidate is permitted to take the end semester examination in the subject in which the candidate does not fulfill the attendance requirement.

4.3 If a student is absent from all the classes without prior permission his/her name will be removed from the rolls of the university.

5. Assessment and Examination:

5.1. Credits:

Credit points will be awarded for all the subjects. One credit is equivalent to ten classroom contact hours.

Each core subject will carry either 6 or 3 credits, and practical courses will carry either 6 or 3 credits depending on the number of hours of teaching and training

5.2. Pattern of Assessment:

Assessment of student's performance will be based on two components i.e, internal assessment and end semester examination conducted at the end of each semester.

A theory subject will comprise of an internal assessment component of 20 marks and an end semester examination component of 80 marks.

A practical subject will comprise an internal assessment component of 20 marks an end semester examination component of 80 marks.

The split of internal Assessment marks for Theory subjects will be as follows:

Criteria	**Maximum Marks**	**Evaluation pattern**
Internal Test	16 (8+8)	(40% Weightage each) based on 2 appropriately spaced class test during the semester(Average of both tests)
Seminar presentation	2	10 % Weightage
Attendance	2	10% Weightage
Total	**20**	

The split of internal assessment marks for practical subjects will be as follows:

Criteria	**Max. Marks**	**Evaluation pattern**
Record / Performance	10	10 % Weightage
Viva voce	10	10 % Weightage
Total	**20**	

The end semester examinations will be conducted as per the university regulations.

5.3. Assessment of project work:

The project work will carry a total of 200 marks. Of this, 150 marks are for the project work and 50 marks for performance in the viva-voce examination

6. Eligibility for pass:

6.1. A student shall be declared to have passed on a semester

(i) If he/she secures a minimum of 50% of marks as semester aggregate;

and

(ii) If he/she secures a minimum of 40% marks in the end semester examination in each paper(Theory and Practical);

And

(iii)If he/she secures a aggregate of 40% marks in each paper including internal assessment.

6.2. A student reappears for the failed in semester in he/she secures less than 50% of marks in semester aggregate. He/she would be required to appear in such papers where he/she has secured less than 50% marks including internal assessment.

6.3. When a student reappears for the failed subject(s), the internal assessment marks originally secured by him/her in the first appearance in the subject(s), if any, will be carried forward.

6.4. Promotion of the student to the next semester, is not automatic, but is dependent on certain other conditions like regularities / attendance / participation activities, discipline etc.

7. Classification of successful students:

7.1. The equivalent of percentage of marks in terms of letter grades and numerical grades in given in the following table. On successful completion of the programme, the students will be classified as below:

Grade	A+	A	B	C	D	E*	F
Corresponding grade point	5.0	4.0	3.5	3.0	2.5	*	0
Percentage of marks	90-100	75-89	70-74	60-69	50-59	*	Less than 50
Class	DISTINCTION		FIRST		SECOND	*	FAIL

- A student who has secured 40% and above but less than 50% marks as aggregate in that paper 50% and above marks in semester aggregate shall be awarded a letter grade E and numerical grade 2.0 in that paper.

7.2. SGPA and CGPA

a) The semester grade point Average (SGPA) is the weighted average of all the grades awarded to a student in a particular semester. The SGPA is computed by dividing the total grade points earned with the total of credits registered in the semester.

b) The cumulative Grade point average(CGPA) is the weighted average of all the grades awarded to a student since the start of the programme up to and including the latest semester.

7.3. Ranks:

Only students, who have passed each of the semester examination at the first appearance, shall be eligible for award of ranks. The first three ranks shall be notified.

8. Award of Qualification:

Students will be awarded the M.Sc microbiology degree upon fulfillment of the following criteria-

a. Must have passed all the subjects of the four semesters;

b. Must have secured a minimum of 50% marks in the project work(Wherever applicable) or a grade point of 2.5 or grade D;

c. Must have complied with all other assessment guidelines and criteria notified during the conduct of the programme.

9. Maximum period for the completion of the programme:

The maximum period for the completion of the programme shall be four years from the date of joining the programme.

10. General guidelines:

10.1. Academic integrity and Ethics

a. A student who has committed an act of academic dishonesty will be deemed to have failed to meet the basic requirement of satisfactory academica performance. Thus, academic dishonesy is not only a basis for disciplinary action but also is relevant to the evaluation of student's level of performance and progress.

b. Where there has been violation of the basic ethos and principles of academic integrity and ethics, the Director/ board of examiners/ course coordinator may use their discretion in terms of disciplinary action to be taken.

c. Academic dishonesty includes, but is not necessarily limited o the following-

i. Cheating or knowingly assisting another student in committing an act of cheating ;
ii. Unauthorized possession of examination materials, destruction or hiding of relevant materials;
iii. Act of plagiarism;

iv. Unauthorized changing of marks or making on examination records.

10.2. Attendance:

a. Students are required to attend and participate in all scheduled class sessions, guest lectures, workshops, learning programs and club / forum activities of both academic and non –academic nature.

b. Students may be discontinued from the programs due to excessive and non –intimated absences.

c. Students may be notify the program coordinator in writing, the reasons for absence, if any, from class sessions, activities and assessment components.

10.3. General:

a. The students are expected to spend a considerable amount of time in research, reading and practice,

b. All students are expected to develop and maintain a positive professional attitude and approach throughout the programme and in conduct of all other activities.

c. Attendance alone is not sufficient. Students are expected to participate, to help the class learn and understand the topics under consideration.

d. Food and drinks are not permitted in the classroom / conference hall.

e. All students expected to dress as per stipulated dress code.

f. Cell phones are strictly prohibited in the campus.

SCHEME OF STUDY AND EXAMINIATONS:

Semester I

Paper No.	**Title of the paper**	**Lecture hours / week**	**Total marks**		
			UE	**C/A**	**Total**
MSc CH 101	Inorganic chemistry	4	80	20	100
MSc CH 102	Organic chemistry	4	80	20	100
MSc CH 103	Physical Chemistry	4	80	20	100
MSc CH 104	Mathematics, computer Science & Env. Chemistry	4	80	20	100
Learning labs					
MSc CH 105	Inorganic chemistry	8	70	30	100
MSc CH 106	Organic chemistry	8	70	30	100
	Total	32	460	140	600

Semester II

Paper No.	**Title of the paper**	**Lecture hours / week**	**Total marks**		
			UE	**C/A**	**Total**
MSc CH 201	Inorganic chemistry	4	80	20	100
MSc CH 202	Organic chemistry	4	80	20	100
MSc CH 203	Physical Chemistry	4	80	20	100
MSc CH 204	Spectroscopy - I	4	80	20	100
Learning labs					
MSc CH 205	Organic chemistry	8	70	30	100
MSc CH 206	Physical Chemistry	8	70	30	100
	Total	32	460	140	600

Semester III

Paper No.	Title of the paper	Lecture hours / week	Total marks		
			UE	C/A	Total
MSc CH 301	Inorganic chemistry	4	80	20	100
MSc CH 302	Organic chemistry	4	80	20	100
MSc CH 303	Physical Chemistry	4	80	20	100
MSc CH 304	Analytical Chemistry - 1	4	80	20	100
Learning labs					
MSc CH 305	Physical Chemistry	8	70	30	100
MSc CH 306	Inorganic chemistry	8	70	30	100
	Total	32	460	140	600

Semester IV

Paper No.	Title of the paper	Lecture hours / week	Total marks		
			UE	C/A	Total
MSc CH 401	Analytical Chemistry – 2	4	80	20	100
MSc CH 402	Spectroscopy – 2	4	80	20	100
Electives (Any two)					
MSc CH 403	Bio Chemistry	4	80	20	100
MSc CH 404	Industrial chemistry	4	80	20	100
MSc CH 405	Nano technology	4	80	20	100
Projects					200

	Total	32	460	140	600

SEMESTER I

MSCCH101

Inorganic Chemistry **55 hrs**

Module 1

Chemical Bonding

Periodic properties of elements, oxidation numbers, octet rule, concepts of resonance and hybridization. VSEPR model, shapes of molecules; bent rules and energetics of hybridization. Electronegativity and partial ionic character; Bonds: covalent, coordinate, multicentre quadruple and Synergic. Hydrogen bonds- types and detection, agostic bond, Intermolecular forces, metallic bond. **9hrs**

Lattice energy, Born-Lande equation, Fajans rules, Slaters rules, radius-ratio rules, structures of simple solids and Zintl isoelectric relationships in solids. MO Theory: σ, π and δ molecular orbital, MOs of diatomic molecules, Electron Angular momentum and classification of states. **8hrs**

Module 2

Chemistry of the Main Group Elements

Periodicity and general trends in properties, polymorphism of carbon, phosphorous and sulphur: properties, structure and bonding in boranes, carboranes, borazines, phosphazenes, phosphonitrilic compounds, sulphur-nitrogen compounds, oxyacids of nitrogen, phosphorous, sulphur and halogens; noble gas compounds. **12hrs**

Module 3

Silicates-classification and structures, isomorphous replacement, pyroxenes, layered

and vitreous silicates, silicate glasses, borosilicate glasses, glass ceramics, silica gel, zeolites and molecular sieves, condensed phosphates, polyhalides. **12hrs**

Module 4

Solvent systems; Bronsted and Lewis acids and bases, pH and pKa, HSAB concept, acid-base concept in non-aqueous media, levelling effect, super acids, reactions in BF_3, N_2O_4. **6hrs**

Isopoly and heteropoly acids and their salts. **4hrs**

Nuclear Chemistry

Sub atomic particles and their properties, nuclear stability, structural models; Liquid drop model and Shell model of the nucleus. **4hrs**

SUGGESTED BOOKS

1. Basic Inorganic Chemistry, F. A. Cotton, G. Wilkinson and P. L. Gaus, John Wiley & sons (1995).
2. Advanced Inorganic Chemistry 3rd, 5th and 6th Editions. F. A. Cotton, G. Wilkinson.
3. Inorganic Chemistry,4th Edition, J. E. Huheey, E. A. Keiter and R. L. Keiter, Addison-Wesley (1993)
4. Inorganic Chemistry, 2nd Edition, D. F. Shriver, P. W. Atkines and C. H.Langford, ELBS (Oxford Uni. Press) (1994).
5. Chemistry of the Elementals, N. N. Greenwood and A. E. Earnshaw, Butterworth Heinemann (1997).
6. Essential Trends in Inorganic Chemistry, D. M. P. Mingos, Oxford Univ.Press (1998).
7. Concise Inorganic Chemistry; 5th Edition; J. D. Lee (1996).

8. Essentials of Nuclear Chemistry, Fourth Edition, H. J. Arnikar, NAIL Pub (1995).

MSCCH102

Organic Chemistry **55 hrs**

Module 1

Stereochemistry

Stereoisomerism: Projection formulae [flywedge, Fischer, Newman and sawhorse], enantiomers, diasteroisomers, mesomers, racemic mixture and their resolution, configurational notations of simple molecules, *DL* and *RS* configurational notations.

Stereoselectivity: Meaning and examples of stereoselective reactions, diastereoselective reactions, stereospecific reactions, regioselective, regiospecific reactions, enantioselective reactions and enantiospecific reactions.

Optical isomerism: Conditions for optical isomerism: Elements of symmetry-plane of symmetry centre of symmetry, alternating axis of xymmetry (rotation-reflection symmetry). Optical isomerism due to chiral centers and molecular dissymmetry, allenes and biphenyls, criteria for optical purity.

Geometrical isomerism: Due to C=C, C=N and N=N bonds, E, Z conventions, determination of configuration by physical and chemical methods. Geometrical isomerism in cyclic systems.

Conformational analysis: Elementary account of conformational equilibria of ethane, butane and cyclohexane. Conformation of cyclic compounds such as cyclopentane, cyclohexane, cyclohexanone derivatives and decalins. Conformational analysis of 1,2-, 1,3- and 1,4-disubstituted cyclohexane derivatives and *D*-Glucose, Effect of conformation on the course andrate of reactions. **18 hrs**

Module 2

Reaction mechanism-I

Structure and reactivity: Brief discussion on effects of hydrogen bonding, resonance, inductive and hyperconjugation on strengths of acids and bases.

Methods of determining organic reaction mechanism: Thermodynamic and kinetic requirements for reactions, kinetic and thermodynamic control. Hammonds postulates and Curtin-Hammett principle.

Identification of products. Formation, structure, stability, detection and reactions of carbocations (classical and non-classical), carbanions, free radicals, carbenes, nitrenes, nitrile oxides, nitrile imines, nitrile ylides and arynes. Determination of reaction intermediates, isotope labeling and effects of cross over experiments. Mechanism of ester hydrolysis. Kinetic and stereochemical evidence, solvent effect. Linear free energy relationship-Hammet equation and Taft treatment. **18 hrs**

Module 3

Reaction mechanism-II

Basics of organic reactions: Meaning and importance of reaction mechanism, classification and examples for each class.

Aliphatic substitution reaction:

Nucleophilic substitution reactions: Kinetics, mechanism and stereochemical factors affecting the rate of $S_N1, S_N2, S_Ni, S_N1', S_N2'$ and S_Ni' reactions, Neighboring group participation.

Electrophilic substitution reactions

Aromatic substitution reactions **10 hrs**

Module 4

Nucleophilic substitution reactions: S_N1, S_N2 and benzyne mechanism, Bucherer reaction.

Electrophilic substitution reactions: Mechanism of nitration, halogenation, sulphonation, Friedel-Crafts alkylation and acylation, Mannich reaction, chloromethylation, Vilsmeier-Haack reaction.

Mechanism of Addition reactions: Addition to C-C multiple bonds involving electrophiles, nucleophiles. Markownikoff's rule and anti-Markownikoff's rule.

Elimination reactions: Mechanism and stereochemistry of eliminations - E_1, E_2, E_1cB. *cis* elimination, Hofmann and Saytzeff eliminations, competition between elimination and substitution, decarboxylation reactions. Chugaev reaction.

Mechanism of hydrolysis of carboxylic acid derivatives: Hydrolysis of esters, amides and acid chlorides. **9 hrs**

References:

1. Organic Chemistry by Morrison and Boyd.
2. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mc Graw Hill, New York, 1987.
3. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. I & II, 1984.
4. E.L. Eliel and S.H. Wilen, Stereochemistry of Organic Compounds, John Wiley and Sons, New York. 1994.
5. Basic Principles of Organic Chemistry by Roberts & Caserio

6. N.S. Issacs, Reactive Intermediates in Organic Chemistry, John Wiley and Sons, New York.1974.
7. R.K. Bansal, Organic Reaction Mechanism, Wiley Eastern Limited, New Delhi, 1993.
8. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
9. A Guide Book to Mechanism in Organic Chemistry by Petersykes
10. Stereochemistry and Mechanism through Solved Problems by P.S. Kalsi.
11. Text book of Organic Chemistry by P.S. Kalsi.
12. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
13. S.K. Ghosh, Advanced General Organic Chemistry, Book and Alleied (P) Ltd, 1998.
14. Organic chemistry, Gram Solomons.

MSCCH103

Physical Chemistry **55 hrs**

Module 1

Thermodynamics

Statistical Thermodynamics

Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging- postulates of ensemble averaging. Canonical, grand canonical and micro canonical ensembles with corresponding distribution laws (using Lagranges method of undetermined multipliers). Fermi-Dirac statistics - distribution law and applications to metal. Bose-Einstein statistics-distribution law and application to helium. Heat capacity behaviour of solids. Heat Capacities of Solids: Einsteins theory of heat capacity of solid, Debye's theory, Characteristic temperature and use of Debye Equation for the determination of heat capacity at low temperature **10 hrs**

Micro and macrostates

Phase space and ensembles. microscopic reversibility and Onsager's reciprocity relations Concept of distribution - thermodynamic probability and most probable distribution - Maxwell-Boltzmann distribution law. Maxwell`s distribution of molecular velocities. Maxwell-Boltzmann statistics and applications, Bose-Einstein and Fermi-Dirac statistics **5hrs**

Module 2

Molecular statistics

distribution of molecular states, deviations of Boltzmann law for molecular distribution, translational partition function, Maxwell-Boltzmann law for distribution of molecular velocities, physical significance of the distribution law, deviation of expressions for average, root mean square and most probable velocities, experimental verification of the distribution law. Molecular collision in gases, mean free path, collision diameter and collision number in a gas and in a mixture of gases, kinetic theory of viscosity and diffusion. **5hrs**

Electrochemistry

Arrhenius theory of strong and weak electrolytes and its limitations, Debye-Huckel theory of strong electrolytes, Debye Huckel-Onsager equation, Debye-Huckel limiting equation for activity coefficients, Debye-Huckel equation for appreciable concentrations. A brief survey of Helmholtz- Perrin, Gouy-Chapman and Stern electrical double layer

(No Derivation). Liquid junction potential and its determination. Transport Number**:** Determination of transport number by Hittorf method and e.m.f method. True and apparent transport numbers. Abnormal transport numbers, effect of temperature and concentration on transport number. Onsagar conductance equation, effect of high electric field and high frequency on ion conductance; surface tension of electrolytic solutions, polyelectrolyte

Irrversible electrode process: Introduction, reversible and irreversible electrodes, reversible and irreversible cells. Polarization, over voltage - ohmic over voltage, concentration over voltage activation over voltage, experimental determination of over voltage. Equations for concentration over potential, diffusion current – stationary current, potential curves, thickness of diffusion layer, diffusion controlled current – potential curves at a dropping mercury electrode, polarography, half wave potential, application in qualitative and quantitative analysis. Energy barrier and electrode kinetics, Butler-Volmer equation, Tafel equation. Hydrogen over voltage and Oxygen over voltage. Effect of temperature, current density and *p*H on over voltage. **14 hrs**

Module 3

PHOTOCHEMISTRY

Absorption of light and nature of electronic spectra, electronic transition, Frank-Condon principle, selection rules, photodissociation, predissociation, photochemical reactions: photoreduction, photooxidation, photodimerization, photochemical substitution, photoisomerization, photochemistry of environment: Green house effect.

Photo physical phenomena: Electronic structure of molecules, molecular orbital, electronically excited singlet states, designation based on multiplicity rule, life time of electronically excited state, electronic transitions and intensity of absorption bands, photphysical pathways of excited molecular system(radiative and non-radiative), prompt fluorescence, delayed fluorescence, and phosphorescence, fluorescence quenching: concentration quenching, quenching by excimer and exciplex emission, fluorescence resonance enrgy transfer between photexcited donor and acceptor systems. Stern-Volmer relation, energy transfer efficiency, examples and analytical significance.

Photochemistry: Introduction to photochemistry, quantum yield and its determination, factors affecting quantum yield, Actinometry -Uranyloxalate and potassium ferrioxalate actinometers, acetone and diethylketone actinometers. Term symbols and significance. Photosensitization: by mercury, dissociation of H2. Photochemical kinetics of: Decomposition of CH3CHO, formation of HCl. Photodegradation: Photocatalyst – ZnO, TiO2, principle, application of ZnO/TiO2 in the photo degradation of dyes (IC), pesticides (DDT) and in industrial effluents. Effect of photo degradation on COD value

Photophysical process: Emission and loss process. Jablonski diagram, quenching and Collisional deactivation, stern-volmer plot. Fluorescence, Phosphorescence, Intramolecular energy transfer (IC and ISC). Intermolecular energy transfer. Lasers, excimer and exciplexes. **14 hrs**

Module 4

Biophysical chemistry

Electrophoresis - principles of free electrophoresis, zone electrophoresis, gel electrophoresis and its applications in qualitative and quantitative study of proteins. Determination of isoelectric point of a protein. Electro osmosis and streaming potential and its biological significance. Biological significance of Donnan membrane phenomenon. Micelles and its involvement during digestion and absorption of dietary lipids. Diffusion of solutes across biomembranes and its application in the mechanism of respiratory exchange. “Salting In” and “Salting out” of proteins. Significance of viscosity in biological systems - mechanism of muscle contraction, detection of intrastrand disulfide bonds in proteins, polymerization of DNA. Effect of temperature and pH on the viscosity of biomolecules (albumin solution). **7 hrs**

SUGGESTED BOOKS

1. Kinetics and mechanism of chemical transformation, J. Rajaraman and J. Kuriacose, Mc Millan, (1986)
2. Molecular thermodynamics, Donald A.Mc Quarrrie, John D.Simon University Science Books, California, (1999).
3. Thermodynamics for Chemists by S. Glasstone, East-West Press, New Delhi, (1960).
4. Thermodynamics, Rajaraman and Kuriacose, East West, 1986.
5. Statistical Thermodynamics, M. C. Gupta (Wiley eastern Ltd.) 1993.
6. Elementary Statistical Thermodynamics , N.D. Smith, Plenum Press, N.Y. (1982).
7. Elements of Classical and Statistical Thermodynamics, L. K. Nash, Addison-Wiley (1970).
1. Modern Electrochemistry- Vol. I and II, J.O.M.Bockris and A.K.N.Raddy, Plenum, New York (1978).
2. An Introduction to Electrochemistry- Samuel Glastone, East-West edition, New Delhi (1942).
3. Text Book of Physical Chemistry- Samuel Glastone, 2nd edition, Mac Millan India Ltd. (1991).

MSCCH 104

Computer Science, Mathematics for Chemists and Environmental Chemistry 55 hrs

Part A- Computer Science (10+5) =15Hrs

Module 1

Introduction to computing

What is computer? Generation of computers, Classification of Computer, Computer Hardware and software, Block diagram of Computer. Input devices, Output devices, Storage devices, Printers, Bits and Bytes, Memory: Primary Memory, Secondary Memory. Definition of operating system. Types of operating system, Function of operating system, Generation of Language, Machine Language, Assembly Language and Higher Level Language.

Data Storage

Data storage: The decimal number system, the binary number system, hexadecimal notation, octal number system. Conversion from one number system to another number system. Codes, ASCII, BCD etc. Arithmetic Operation for Binary Numbers: addition, subtraction, multiplication, and division. Representation of numbers in 1's and 2's Complement method. Subtraction using 1's and 2's Complement method.

Data Manipulation

Logical Operations: AND, OR, NOT, NANT, NOR, EX-OR, EX-NOR. Logic gates with truth table, Universal Gates, Representation of function using gates. Boolean algebra: Postulates, Minimization of functions.

Module 2

Computer applications

The students will be taught to operate a PC and how to run standard programs and packages such as MS-WORD, EXCEL, ORIGIN, SIGMA PLOT, CHEM SKETCH etc. and solve chemistry problems. Problems will be taken preferably from physical chemistry for plotting first and second derivative curves, linear plots etc. Problems from chemical kinetics, polymer chemistry, analytical chemistry, electrochemistry, spectroscopy etc. will be solved.

Computational Chemistry

Fortran/C Programming and numerical method feature of fortran C : Basic theory a)Solution of equation: Bisection, regular tabs, Newton – Raphion and related method forsolving polynomical and trancendented equation, convergence. b) Liner simultaneous equation: Gaussion alimination, Gauss – seidel method, Gauss jorden method. Fivolting strategy, errors and ill c) Numerical Differentiation: Solution of simple differential equation by Tegler seies and Rurge – Kutta methods. d) Numerical Differentiation: Newton – coted formulae, Romberg integration, errors in integration formulae .Internet: Introduction to networking and search using Internet. Running of advanced scientific packages. Project: The student will develop utilities such as analysis of spectra, simulation programs which will supplement laboratory of theory exercises in Physical, Organic, Inorganic and Analytical chemistry.

Recommended Books:

1. Computational Chemistry, A.C.Norris, John Wiley.
2. Computer Programming in FORTRAN 77, Rajaraman, Prentice Hall.
3. Numerical Analysis, C.E.Frogberg, Macmillan.
4. Numerical Analysis, A Practical Approach, M.J. Maron, John Wiley.
5. Numerical Methods for Scientists and Engineers, H.M.Anita, Tata McGraw Hill.
6. Computers in Chemistry, K.V. Raman
7. Computers and their applications to Chemistry, Ramesh Kumari, Narosa

Part B – Mathematics for Chemists (10Hrs)

Module 3

Vectors: vectors dot and cross products: scalar and vector triple products and their applications ,tensors and their applications.

Matrix Algebra: Review of different types of matrices (including Hermitian and skew-Hermitian) matrix addition and multiplication; determinant of a square matrix, transpose, adjoint and inverse of a square matrix. Solution to system of linear equations (a) by matrix, method & (b) by Cramer's rule .

Characteristic equation of a square matrix, eigen values and eigen vectors.

Calculus: Rule for differentiation; Chain Rule (for $f(X) = U^n$, sin u, log u etc.) implicit differentiation and parametric differentiation and successive differentiation of order 2.(for explicit functions only).

Applications of differentiation – derivative as a slope of the tangent, derivative as a rate measure – velocity and acceleration, increasing and decreasing functions- maxima and minima –second derivative test- point of inflections-problems restricted to polynomials.

Integration: Basic rules – simple substitution-Method of partial fractions –Integration by parts. Definite integral and application to areas of plane curves.

Functions of several variables; partial derivatives; co-ordinate transformation from Cartesian co-ordinates to spherical and cylindrical co-ordinates and vice-versa.

Elementary Differential equation: variable separable, exact first order equations, linear and homogenous equation.

Second order homogenous differential equation with constant coefficients; f(D)y=0.Solution of differential equations by power series method.

Fourier series: Simple problems.

Probability: Review of permutations and combinations. Probability and addition theorem for mutually exclusive events and multiplication theorem for independent events.

Curve Fitting- method of least squares.

SUGGESTED BOOKS

1. Calculus and analytical geometry thomas. Finney. Narosa publishing house.

2. Short course in differental equations .rainville and bedient, ibh publishers.
3. Theory and problems in mathematics,vol ii ,s.s. bosco,
4. Algebra-hall and Knight.
5. Mathematics for Chemistry, Doggett and Suchffe, Longmann Publishers.
6. Mathematical preparation for physical chemistry, F.daniels, Mcgraw Hill.
7. Chemical Mathematics, D.M. Hirst, Longman publishers.
8. Basic Mathematics for chemists.Tebbutt, Wiley publishers.

Part C - Environmental Chemistry (25Hrs)

Module 4

Natural resources

Water Resources, Availability, Use of Water, Water Quality, Water Quality Parameter and Standrads, Most Probable number (MPN), Water Borne Diseases and Water Induced Diseases, Other Water Induced Diseases, Fluoride Problem in Drinking Water, Mineral Resources, Metallic Resources, Non-Metal Resources, Material Cycles, Carbon Cycle, Nitrogen Cycle, Sulphur Cycle. **6hrs**

Energy

Introducation, Different Types of Energy, Fossil Fuel, Nuclear Fission and Nuclear Fusion,Nuclear Fission, Nuclear Fusion, Solar Power, Solar Heating Systems, Photovaltaic Systems, Wind Energy, Demerits, Hydro Energy, Merits, Other Hydro Sources, Bio Energy, Sources of Bio energy, Hydrogen as an alternative fuel, Scope, Fuels, Electro Magnetic Radiation (EMR), Electro Magnestic Spectrum, Comparison of various forms of Energy. **7hrs**

Environmental concerns

Acid rain, Introducation, Definitioin, Causes of acid rain, III effects some historical evidences, Control of acid rain, Ozone depletion, Introducation, What is ozone? What is UV radiation?, Formation of ozone in stratosphere, What is ozone depletion or making a hole in the sky?, Causes of ozone depletion, Control measures, Animal husbandry. **5hrs**

MSCCH105

Inorganic Chemistry practicals

(4 days a week 4 ½ hours a day)

A. Semi-micro qualitative analysis of mixtures containing two each of common cations and anions and one of the rare earth metals.

Inorganic Mixtures

1. $CdSO_4$+ Potassium titanium oxalate.
2. Potassium titanium oxalate +$ZnSO_4$.
3. Zinc Nitrate+ sodium borate + Barium borate.
4. Lead acetate + $MnSO_4$ + Lithium acetate.
5. Zirconium nitrate + sodium borate + stronsium nitrate
6. Sodium molybdate + barium borate + Na_2SO_4
7. Sodium molybdate + sodium borate + aluminium sulphate.
8. Bismuth carbonate + zinc carbonate + lithium acetate.
9. Cadmium carbonate + $CaCO_3$ + Lithium acetate
10. Cadmium phosphate + aluminium sulphate + lithium sulphate.
11. Potassium titalium oxalate + $MnSO_4$.
12. Zirconium nitrate + cadmium phosphate + sodium nitrite.
13. Bismuth carbonate + Potassium titanium oxalate.
14. Sodium molybdate + aluminium sulphate + Na_2SO_4 +oxalic acid.

B. Preparation and Quantitative analysis of inorganic complexes

15. Ferrous oxalate
16. Potassium trioxalatoferrate(III) trihydrate.
17. Hexammine cobalt (III) chloride.
18. Cis and trans-potassium dioxalatodiaquochromium(III).

MSCCH106

Organic chemistry practical

PART – IIA

1. Preparation of *p*-nitro aniline from acetanilide.
2. Preparation of n-butyl bromide from n-butanol.
3. Preparation of *p*-nitroiodobenzene from paranitroaniline.
4. Preparation of aniline from nitrobenzene.
5. Preparation of ß-*D*-Glucose penta acetate.
6. Preparation of phenoxy acetic acid.
7. Preparation of cyclohexanone from cyclohexanol.
8. Preparation of chalcone.
9. Preparation of *S*-benzylthiuronium chloride.
10. Condensation of anthracene and maleic anhydride (Diels-Alder reaction).
11. Preparation of *m*-nitrobenzoic acid from methyl benzoate
12. Separation of amino acid by paper chromatography.

PART – IIB

Qualitative analysis: Separation of binary mixtures, identification of functional groups and preparation of suitable solid derivatives.

References:

1. Manual of Organic Chemistry - Dey and Seetharaman.
2. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
3. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.
4. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
5. Practical Organic Chemistry - Mann & Saunders
6. Semimicro Qualitative Organic Analysis by Cheronis, Entrikin and Hodnet .

7. R.K. Bansal, Laboratory Manual of Organic Chemistry, New Age International (P) Ltd. London, 3rd edition, 1996.

SEMESTER II

MSCCH 201

Inorganic Chemistry

55 Hrs

Inorganic Chemistry-II (Co-Ordination Chemistry)

Module 1

Metal-Ligand Equilibria in Solution

Step-wise and overall formation constant and their relationship, trends in step-wise constant, kinetic and thermodynamic stability of metal complexes, factors affecting the stability of metal complexes with reference to the nature of the metal ion and ligand, chelate and macrocylic effects and their thermodynamic origin, determination of binary formation constants by pH-metry, spectrophotometry, polarography, and by ion exchange methods **12hrs**

Module 2

Metal-Ligand Bonding

Crystal field theory-limitation, stereochemistry, coordination Nos,3 to 8, Evidences for metal-ligand orbital overlap, MO theory (including π- bonding), Jahn-Teller distortion in metal complexes and metal chelates, Spectrochemical series, Nephelauxetic series, angular overlap model. 10 **hrs**

Module 3

Structure and Bonding-Hydride, dihydrogen, simple metal carbonyl, Nitrosyl, dinitrogen and tertiary phosphine complexes, metal complexes as liquid crystals, stereo chemical non-rigidity, self-assembly in supramolecular chemistry; Stereoisomerism-

chirality, optical activity, CD, ORD, Cotton effect and magnetic circular dichroism, absolute configurations **14hrs**

Module 4

Electronic Spectra of Transition Metal Complexes.

Spectroscopic ground states, selection rules, term symbols for d^n ions, Racah parameters, Orgel correlation and Tanabe-Sugano diagrams, spectra of 3d metal aqua complexes of trivalent V,Cr, divalent Mn, Co and Ni, $[CoCl_4]^{2-}$, calculation of Dq, B and β parameters, charge transfer spectra. **12hrs**

Magnetic Properties of Metal Complexes

Magnetic susceptibility, types of magnetic behaviour, diamagnetic corrections, orbital contribution, spin-orbit coupling, Ferro and antiferromagnetic coupling, spin crossover.

7hrs

SUGGESTED BOOKS

4. Basic Inorganic Chemistry, F.A. Cotton, G.Wilkinson and P.L.Gaus, John Wiley & sons Inc, 6th Edition (1999)
5. Inorganic Chemistry,4th Edition, J.E. Huheey, E.A.Keiter and R.L.Keiter, Addison-Wesley (1993)
6. Inorganic Chemistry, 2nd Edition, D.F. Shriver, P.W.Atkins and C.H.Langford, ELBS (Oxford Uni. Press) (1994).
7. Chemistry of the Elementals, N.N. Greenwood and A.E.Earnshaw, Butterworth Heinemann (1997).
8. Inorganic Electronic Spectroscopy, A.B.P.Lever, Elsevier.
9. Essential Trends in Inorganic Chemistry , D.M.P.Mingos, Oxford Univ.Press(1998).

10. Magnetochemistry, R.L. Carlin, Springer Verlag.
11. Electronic Absorption Spectroscopy and Related Techniques, D.N. Sathyanarayana , Universities Press (2001).

MSCCH 202

Organic chemistry

55 hrs

Reagents in organic synthesis, photochemistry and pericyclic reactions

Module 1

Reductions: Catalytic hydrogenations (homogeneous and heterogeneous) - catalysts, solvent, equipment and reduction of functional groups, catalytic hydrogen transfer reactions. Wilkinson catalyst. Bakers yeast, $LiAlH_4$, $NaBH_4$, metal dissolving reactions (Birch reduction). Leukart reaction (reductive amination), diborance, Meerwein-Ponndorf-Verley reduction, Wolf-Kishner reduction, Clemensen reduction.

Oxidations: Oxidation with chromium and manganese compounds (CrO_3, $K_2Cr_2O_7$, PCC, PDC, Sarret reagent, Jones reagent, MnO_2, $KMnO_4$), oxygen (singlet and triplet), ozone, peroxides and peracids, lead tetra acetate, periodic acid, OsO_4, SeO_2, NBS, chloramine-T, Sommelet oxidation, Oppenauer oxidation. **18 hrs**

Module 2

Reagents in organic synthesis: Use of following reagents in organic synthesis and functional group transformations: Lithium disopropylamide (LDA), Gilmann reagent, dicyclohexyl carbodimide (DCC), dichloro dicyano quinone (DDQ), phase transfer catalyst, crown ethers, Fenton's reagent, Ziegler-Natta catalyst, diazomethane, stannous chloride, Sharpless epoxidation, Woodward and Prevost hydroxylation, Stark enamine reaction, Phosphorus ylides – Wittig and related reactions, 1,3-dithiane anions - Umpolung reaction, sulphur ylides – reactions with aldehydes and ketones, Peterson reactions - synthesis of alkenes.

Organometallic chemistry, introduction, types, classification, Homogeneous catalysis, Alkene hydrogenation, hydroformylation, Wacker's process, Monsanto acetic acid process and L-DOPA synthesis, Alkene oligomerizations, Water-gas shift reactions.

18 hrs

Module 3

Photochemistry and concerted reactions: Introduction, light absorption and electronic transitions, Jablonski diagram, intersystem crossing, energy transfer, sensitizers, quenchers.

Photochemistry of olefins, conjugated dienes, aromatic compounds, ketones, enones, photooxidations, photoreductions, Norrish type I and II reactions, Paterno-Buchi reaction, Barton reaction, Di-pi-rearrangements.

Electrocyclic reactions: Stereochemistry, symmetry and Woodward-Hofmann rules for electrocyclic reactions, FMO theory of electrocyclic reactions, correlation diagram for cyclobutadiene and cyclohexadiene systems.

Module 4

Cycloaddition reactions: Classification, analysis by FMO and correlation diagram method. **1,3-dipolar cycloadditions**: involving nitrile oxide, nitrile imine, nitrile ylide cycloaddition. Intra and intermolecular 3+2 cycloaddition and their application in organic synthesis. **[4+2] cycloaddition reactions**: Deils-Alder reacion, hetero Diels-Alder reaction and their applications.

Sigmatropic reactions: Classification, stereochemistry and mechanisms. suprafacial and antarafacial shifts of H, sigmatropic shifts involving carbon moieties. [3,3] and [5,5]-sigmatropic rearrangement, Claisen, Cope and aza-Cope rearrangement **19 hrs**

References:

1. H. Pine, Hendrickson, Cram and Hammond, Organic Chemistry, Mac Grow Hill, New York, 1987.

2. Organic Chemistry - Morrison and Boyd
3. Organic Chemistry- Crabtree
4. Organic Chemistry- Clayden
5. I.L. Finar, Organic Chemistry, ELBS Longmann, Vol. 1 & II, 1984.
6. J. March, Advanced Organic Chemistry, Wiley Interscience, 1994.
7. E.S. Gould, Mechanism and Structure in Organic Chemistry, Halt, Rinhart & Winston, New York, 1964.
8. F.A. Carey and Sundberg. Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York. 1990.
9. Principles of Organic Synthesis - ROC Norman and Coxon.
10. S.K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd. 1998.

MSCCH 203

Physical Chemistry

55 hrs

Module 1

Phase Rule Studies

Application of phase rule to the two component systems- compound formation with congruent melting point and incongruent melting points, Roozeboom's classification. Application of phase rule to three component systems. Systems of three liquids. Phase rule - Derivation of phase rule from the concept of chemical potential, application of phase rule to three component systems. **8hrs**

Corrosion

Manifestations of corrosion, types of corrosion, basis of electrochemical corrosion, theories of corrosion. Local cell theory (Wagner and Traud theory) Current –potential relations (Evan diagram) in corrosion cells. Effect of pH, nature of metal and dissolved oxygen (principle of differential aeration) on corrosion. Corrosion inhibition and prevention by painting, phosphating and by using biomaterials, corrosion protection by anodic (passivation) and cathodic protection.

Corrosion and its prevention

About corrosion: Theories and mechanism of corrosion – thermodynamic and kinetic approaches to the study of corrosion – methods of determination of corrosion rates – Tafel extrapolation, linear polarization and impedance techniques.

Methods of corrosion prevention: Cathodic and anodic protection – corrosion inhibitors.

Passivity: Characteristics – Flade potential – theories and mechanism of passivation – trans-passivity – use of ellipsometric technique in the study of passivating films.

8hrs

Module 2

Macromolecules

3. Chemistry of polymerization: Polymers-definition, types of polymers, liquid crystal polymers. Free radical polymerization(Initiation, propagation and termination), kinetics of free radical polymerization, step growth polymerization(Polycondensation), kinetics of step polymerization, cationic and anionic polymerization.

Mechanism of polymerization, molecular weight of a polymer (Number and mass average) viscosity average molecular weight, numerical problems. Degree of polymerization and molecular weight, methods of determining molecular (05) weights(Osmometry, viscometry, light scattering, diffusion and ultracentrifugation, viscosity, diffusion, light scattering, and sedimentation methods) Molecular mass-number and mass average molecular mass,

Polymer Chemistry: Transitions in polymers: Definition of glass transition temperature (Tg) and flow temperature (Tf) and melting temperature (T), thermal behaviour of amorphous and crystalline polymers, factors affecting the T g. m g Plasticizers, properties and their effect on T of PVC and diethylhexylsuccinate, efficiency of plasticizers, comparison of T copolymers and polymer blends, relation between T g and T m g and T. Preparation, properties and commercial importance: Vinyl polymers: polyethylene, polypropylene, polystyrene, polymethylmethacrilate, polyvinyl chloride, polytetrafluoroethylene. Polyesters: poly(ethylene terephthalate). Polyamides: aramides (Kevlar and Nomex). Polyimides, Polysulphone. Polyurethanes. Polyureas. Natural polymers: polyisoprenes, chitosan. **13hrs**

Module 3

Catalysis

Theory of Homogeneous and heterogeneous catalysis, autocatalysis, oscillatory reactions, (general introductions only), redox reactions, preliminary idea of inner sphere and outer sphere reactions of transition metals.

General catalytic mechanism, Acid-Base catalysis, specific acid and base catalysis. General acid and base catalysis. Mechanism of acid-base catalysis (protolytic and prototropic). Bronsted catalytic law Oxidation of amino acids and carbohydrates in pressence of acid and base catalysis. Acidity functions - Bronstead, Hückel, Hammett and Bunnett hypothesis.

Enzyme kinetics: Catalysis by enzymes - rate of enzymes catalysed reactions - effect of substrate concentration (Michaelis Menton equation),, pH and temperature on enzyme catalysed reactions - inhibition of enzyme catalysed reactions, comparison of enzyme with chemical catalysts, mechanism (lock and key theory), Henri-Michaelis-Menten treatment, significance of Michaelis constant, Lineweaver-Burk plot. Mechanism of single substrate reactions, Competitive, Noncompetitive and Uncompetitive Inhibition. A brief kinetic and mechanistic applications of glucose oxidase in the oxidation of glucose.

13hrs

Module 4

Battery

Energetics of cell reactions: Effect of temperature, pressure and concentration on energetics of

cell reactions (calculation of ΔG, ΔH and ΔS). Electrochemical energy sources – Batteries,

classification, characteristics, primary, secondary and lithium batteries.

Basic Concepts, Electrochemical Principles and Reactions, Primary Batteries—Introduction, Zinc/ Air Batteries, Lithium Batteries, Carbon Anodes

, Oxide Cathodes,, Liquid Electrolytes, Ionic Liquids , introduction, properties, General applications for Lithium-Ion and Related Batteries, Lithium-Ion Secondary Batteries with Gelled Polymer Electrolytes

Solid-Electrolyte Batteries, Secondary Batteries—Introduction, Lead-Acid Batteries, Industrial and Aerospace Nickel-Cadmium Batteries, Advanced Batteries for Electric Vehicles and Emerging Applications—Introduction, Metal/ Air Batteries, Portable Fuel Cells, Introduction

Fuel cells: Classification – alkaline fuel cells, solid polymer electrolyte fuel cells, phosphoric acid fuel cells, molten carbonate fuel cells and solid oxide fuel cells – brief description, reactions and applications of each type of fuel cell**.** **13hrs**

SUGGESTED BOOKS

1. An introduction to Metallic Corrosion and its Prevention by Rajanarayan, Oxford & IBH Publishing Co.,New Delhi(1983).
2. Chemical and Electrochemical Energy Systems by Narayan & Viswanathan, Hyderabad, Universities Press (India) Ltd.,(1998).
3. Corrosion Engioneering by Mars Fontanna, 3rd ed., McGraw Hill, New York (1987).
4. Fuel Cells by Bockris & Srinivasan, John Wley & Sons (1972).
5. Lithium battery technology by H. V. Venkatasetty, John Wiley & Sons Inc.,(1984).
6. Electrochemical Methods – Fundamentals and Applications, 2nd ed. By A, J. Bard and L. R. Faulkner, John Wiley & Sons Inc., New York (2001).

MSCCH 304

Spectroscopy I

55 hrs

Module 1

Molecular Symmetry and Group theory

Concepts of Groups, Sub-groups, Classes of Symmetry operations, Group Multiplication Tables. Abelian and non-Abelian point groups. Symmetry criterion of optical activity, symmetry restrictions on dipole moment. A systematic procedure for symmetry classification of molecules.

Representation of Groups: Matrix representation of symmetry operations, reducible and irreducible representations. The Great Orthogonality Theorem. Construction of character tables for point groups C2v, C3v and D2h, structure of character tables, determination ofsymmetry species for translations and rotations; Mulliken's notations for irreducible representations, reduction of reducible representations using reduction formula, group subgroup relationships, descent and ascent in symmetry, correlation diagrams showing relationship between different groups. Symmetry adapted linear combinations, symmetry aspects of MO theory, sigma- and pibonding in AB4 (tetrahedral) molecule. Molecular symmetry, Representation of symmetry operation as matrices. Definition ofgroups, set of symmetry operations of molecules satisfying the condition of point groups. Representation, basis of representation, reducible and irreducible representation. The great orthogonality theorem, character tables and their applications to chemical bonding.

Symmetry elements,Symmetry operations and point group. Determination of point group.Construction of group multiplication tables. Symmetry species and character tables.Reducible and irreducible representations. Analysis of reducible representations. Number ofnormal modes of vibrational symmetry types. Rule of mutual exclusion. I.R.and Raman active fundamentals. **15hrs**

Module 2

Microwave Spectroscopy

Introduction: Interaction of light with matter, mechanism of absorption & emission of radiation.

Microwave spectroscopy: Classification of molecules; rigid rotor model; rotational spectra of diatomics and polyatomics; effect of isotopic substitution and nonrigidity; selection rules and intensity distribution. Gaseous microwave spectra and rotational transitions : Study of inversion of ammonia andhindered rotations in molecules. Instrumentation. Stark effect in molecular spectra; first andsecond order Stark efects. Rotation - vibration spectra, shapes of absorption bands in case of (i) linear, (ii)symmetrictop, (iii) spherical top and (iv)asymmertic top, molecules. Isotopic effects.

5hrs

Infrared Spectroscopy

Effect of anharmonicity; Morse potential; Vibration-rotational spectra of diatomics; P.Q,R branches, normal modes of vibration, overtones, combination bands and hot bands., Vibrational coupling, qualitative and quantitative analysis, advantages and limitations of quantitative IR methods**.** Structural studies (involving IR and Raman spectroscopy) of coordination compounds containing the following molecules/ions and ligands - NH3, H2O, OH–, $SO4^{2-}$, CN–, SCN–, NO, O2, PR3 and halides. Instrumentation including FTIR.
5hrs

Module 3

Raman spectroscopy

Origin; rotational and vibrational Raman spectra of diatomics. Theory, relation with I R spectroscopy, resonance Raman stimulated hyper and inverse Raman effects. Experimental techniques, structure determination from I R and Raman spectra. Theories of Raman Effect, Concept of polarizibility and polarizibility ellipsoid. Vibrational Raman Spetcra, Rotational raman Spectra of Molecules. Symmetry selection rule and prohibition of inter combination. Influence of nuclear spin in case of homonuclear diatomic molecules. Principle of mutual exclusion, polarization of Raman lines and ortho- and para- modifications. An introduction to laser resonance Raman spectroscopy. Elucidation of structure of molecules, e.g.H_2O, N_2O, CO_2 by Raman Spectra.
5hrs

Electronic Spectroscopy

Basic principle, Hyperfine splittings (isotropic systems); the g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Anisotropic effects (the g-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes. Electronic spectroscopy: Electronic spectra of diatomic molecules, Franck-

Condon principle, Vibronic transitions, Spectra of organic compounds, $\pi \rightarrow \pi^*$, $n \rightarrow \pi^*$ transition. Lasers: Laser action, population inversion, properties of laser radiation, examples of simple laser systems. Electronic spectroscopy of diatomic molecules. Born-Oppenheimer approximation. Vibrational course structure of electronic transitions: The v' and v" progressions. Deslandres table. Intensity: the Franck-Condon principle. Pre dissociation.

5hrs

Module 4

NMR spectroscopy

Chemical shift, Factors affecting chemical shift, Chemical and magnetic equivalence, Spin-spin coupling, Coupling constant J, Factors affecting J, Karplus equation Karplus curve, variation of coupling constant with dihedral angle,, Geminal, vicinal and long range coupling (allylic and aromatic). 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, four and interacting nuclei (first order spectra); Complex interaction, virtual coupling, stereo chemically hindered rotation, nuclear magnetic double resonance, NMR spectroscopy in the structural assessment of inorganic compounds. Nuclear spin and nuclear spin states in magnetic field, resonance phenomenon, relaxation processes, shielding and de-shielding of magnetic nuclei, spectra of a two-spin system (A2, AB and AX cases) Magnetic properties of nuclei, population of energy levels, the Larmar precession, relaxation processes, Chemical shift, shielding mechanism, spin-spin interactions, effect of chemical exchange on spectra. 1H nmr spectra of organic molecules and complex metal ligands, Spectra of paramagnetic complexes, contact shift, double resonance technique, Instrumentation including FT nmr. Equivalence of protons- chemical and magnetic equivalence. Spin-systems First order and second order patterns. Proton attached to elements other than carbon. Exchange phenomena, Temperature effects. Introductory aspects of 15N, 19F, 31P - NMR. Correlation NMR Spectroscopy: Theory, Pulse sequences. FT-Methods. 1H - 1H (COSY)

, 13C – H (HETEROCOSY) and Two-dimensional NMR spectroscopy COSY, NOESY, INDOR, SPI, DEPT Spectra, CIDNP technique, MRI., Complex NMR Spectra: Simplification of complex spectra-isotopic substitution, increased magnetic field strength, double resonance and lanthanide shift reagents; variable temperature probe. 13C-NMR Spectroscopy**:** Comparison of ^{1}H-NMR and ^{13}C-NMR, multiplicity-Proton decoupling-Noise decoupling-Off resonance decoupling-Selective proton decoupling-Chemical shift, application of CMR. Applications of NMR: Structural diagnosis, conformational analysis, keto-enol tautomerism, H bonding. NMR to solids. **10hr**

Mass spectrometry

Molecular ion peak, base peak, isotopic abundance, meta stable ions. Nitrogen rule, Determination of molecular formula of organic compounds based on isotopic abundance and HRMS Fragmentation pattern in various classes of organic compounds (including compounds containing hetero atoms), Retro-Diels-Alder reaction, ortho effect. Recapitulation, instrumentation, ion sources for molecular studies, electron impact, field ionization, field absorption, chemical ionization and fast atom bombardment sources. Mass analyzers: quadrupole, time of flight and ion trap. Applications, use of mass spectrometer as a detector in chromatography**.** Instrumentation, methods of ionization, EI, CI, DI, SI – Methods. Fragmentation: principles, odd and EE ions, molecular ion and base peak, Nitrogen rule,metastable ions. Isotope effects in chloro and bromo compounds. Stevenson rule.Fragmentation of: i) Normal and Branched Alkanes. ii) Alkenes. iii) Benzene and its derivatives. iv) Alcohols. v) Aldehydes. vi) Ketones. vii) Acids. viii) Esters. ix) Ethers. x) Amines.xi) Nitro compounds. xii) Halo compounds. xii) Peptides McLafferty and McLafferty + 1 rearrangement. Calculation of molecular formula. Composite problems: Calculation of H- deficiency Index.

5hrs

Structure determination involving individual or combined use of the above spectral techniques.

4 hrs

Reference Books

1. K. Nakamoto. Infrared and Raman Spectra of Inorganic and Coordination Compounds, (5th edn.), John Wiley (1997).

2 .R. V. Parish. *NMR, NQR, EPR and Mossbauer Spectroscopy in Inorganic Chemistry*, Ellis Horwood, New York (1990).

3. C. N. Banwell & E. M. McCash. *Fundamentals of Molecular Spectroscopy*, Tata McGraw- Hill, New Delhi (2006).

4. R. M. Silverstein, G. C. Basseler & T. C. Morill. *Spectroscopic Identification of Organic Compounds*, John Wiley (1981).

5. W. Kemp. *Organic Spectroscopy* (3rd edn.), McMillan Press Ltd. (1991).

6. D Williams & I. Fleming. *Spectroscopic Methods in Organic Chemistry*, McGraw Hill (1989).

7. Chemical Applications of Group Theory 2nd Edn-F. A. Cotton, Wiley Eastern Ltd (1976).

8. Symmetry and Spectroscopy of Molecules-K. Veera Reddy New Age International, (1998).

9. An introduction to Molecular Spectroscopy by G. M. Barrow, McGraw Hill, New York.

10. Electron Absorption Spectroscopy and Selected Techniques-D. N. Satyanarayana, University Prof. India Ltd. Hyderabad.

11. Introduction to Spectroscopy – by D.L.Pavia, G.M.Lampman and G.S.Kriz, Saunders Golden Sunburst Series London, (1979).
12. Applications of Absorption Spectroscopy of Organic Compounds – by J.R Dyer

13. Interpretation of Mass Spectroscopy – by McLafferty.

14. Spectroscopy of Organic Compounds – by P.S. Kalsi, 4th Edition, New Delhi (2005).

15. Microwave Spectroscopy-J.M. Sugden and C.N. Kenny.

16. Absorption Spectroscopy-R.P.Bauman, Wiley New York, 1952.

17. Introduction to Photoelectron Spectroscopy - P.K.Ghosh., John Wiley

18. D. N. Sathyanarayana, Electronic Absorption Spectroscopy and Related Techniques (2001), Universities Press (India) Ltd., Hyderabad.

19. F. A. Cotton, Chemical application of group theory, Weily eastern

20. Elements of X-ray diffraction, B.Dcullity, Addison Wisley, 1967.

MSCCH 205

Organic practical

PART –IIIA

Isolation of natural products

1. Fractional crystallization: separation of mixture of naphthalene and biphenyl

2. Fractional distillation: Separation of mixture of hexane and toluene.
3. Thin layer chromatography: Separation of plant pigments
4. Column chromatography: Separation of mixture of *o* and *p*-nitro anilines
5. Isolation of piperine from pepper
6. Isolation of caffeine from tea
7. Isolation of azeleic acid from castor oil
8. Estimation of sugars by Fehlings method
9. Isolation of Lycopene and enzymes like Lipase and Sucrase
10. Estimation of sugars by Bertrand's method

PART IIIB

MULTI STEP SYNTHESES AND ESTIMATION OF ORGANIC COMPOUNDS.

1. Molecular rearrangement:
   i. Preparation of *o*-chlorobenzoic acid from phthalic anhydride
   ii. Preparation benzilic acid from benzaldehyde
   iii. Preparation of *o*-hydroxy benzophenone from phenyl benzoate via Fries rearrangement

Prepartion of benzanilide from benzophenone oxime via Beckmann rearrangement

2. Oxidation of cyclohexanol to adipic acid via cyclohexanone
3. Esterification: Preparation of benzoccaine from *p*-nitrotoluene
4. 2-Carbethoxycyclopentanone from Adipic acid
5. Separation of components from mixture of organic compounds by fractional crystallization, fractional distillation, adsorption, Paper and TLC. Their purification and characterization.

6. Determination of enol content by Meyer's method
7. Estimation of ketones by haloform reaction
8. Estimation of nitro groups

References:

8. Manual of Organic Chemistry - Dey and Seetharaman.
9. Modern Experimental Organic Chemistry by John H. Miller and E.F. Neugil, p 289.
10. An Introduction to Practical Organic Chemistry - Robert, Wingrove etc.
11. A Text Book of Practical Organic Chemistry – A.I. Vogel, Vol.III
12. Practical Organic Chemistry - Mann & Saunders
13. Semimicro Qualitative Organic Analysis by Cheronis, Entrikin and Hodnet .
14. R.K. Bansal, Laboratory Manual of Organic Chemistry, New Age International (P) Ltd. London, 3rd edition, 1996.

MSCCH 206

Physical Chemistry Practical

1. Determination of the velocity constant, catalytic coefficient, temperature Coefficient, $t_{½}$ and energy of activation for the acid hydrolysis of methyl acetate.
2. Evaluation of Arrehenius parameters for the reaction between potassium persulphate and potassium iodide (I^{st} order).
3. To study the kinetics of saponification of ethyl acetate by conductivity method, determination the energy of activation.
4. Kinetics of oxidation of glycine by chloramines -T - determination of order with respect to Glycine
5. Test for the validity of Beer – Lambert Law and determination of the unknown concentration of solution. Calculation of molar extinction coefficient.
6. Titration of ferrous ammonium sulfate with potassium permanganate colorimetrically.
7. Determination of concentration of Fe by spectrophotometric titration using EDTA.
8. Spectrophotometric titration of FeSO4 against KMnO4.
9. Conductometric titration of a mixture of HCl and CH3COOH against NaOH.
10. Conductometric titration of a mixture of HCl, CH3COOH and CuSO4 against NaOH.
11. Determine the rate constant of saponification of methyl acetate conductometrically.
12. Determination of dissociation constant of a weak acid by potentiometric method.
13. Potentiometric titration of AgNO3 vs KCl.
14. Equivalent conductance of a weak electrolyte at different concentrations and the applicability of Ostwald's law.
15. Verification of the Onsagar equation for strong electrolytes.
16. Equivalent conductance of a weak electrolyte from Kohlrausch's law.
17. Determination of pH of buffers by using quinhydrone electrode and comparison of the pH values obtained with glass electrode.
18. Detection of proteins using polyacrylamide gel electrophorasis method.

Semester III

MSCCH 301

Inorganic chemistry

52 hrs

Inorganic reaction mechanisms & bioinorganic chemistry

Module 1

Kinetics and mechanism

Labile, inert, stable and unstable complexes; Classification of mechanisms – energy profile of a reaction, experimental evidences in octahedral substitution. Mechanism of ligand substitution in octahedral complexes – kinetics, leaving group, chelate and metal effects, Acid and Base catalysis; acid catalyzed aquation and anation reactions, base hydrolysis, conjugate base hydrolysis, Stereochemistry of octahedral substitution, substitution in trans complexes.

Substitution in square planar complexes: Trans effect, trans influence, theories of trans effect, cis effect, effect of leaving group and entering nucleophile, solvent effects.

Electron transfer reactions: complementary and non-complementary, outer- sphere electron transfer, Marcus equation. Inner-sphere electron transfer – one and two electron transfer reactions, electron transfer through extended bridges, mixed valence compounds, unstable intermediate oxidation states. Oxidative addition and reductive elimination reactions, Isomerization, migratory insertion, chelate effect. Reactions of coordinated ligands, template reactions. Photochemical reactions of cobalt, rhodium, chromium and ruthenium complexes. **20 hrs**

Module 2

Introduction to Bioinorganic chemistry

a. Essential and trace elements in biological processes, elements in biological cell, biomolecules associated with metal ions and their roles.
b. Molecular mechanism of ion transport across cell membranes, Na^+/K^+ ion pump.
c. Metal ion storage and transport-ferritin, transferrin and siderophores.
d. Metal ligand interactions with DNA.
e. Metal ion deficiency, toxicity, detoxification, chelation therapy. Metal complexes in medicine: metal complexes used as anticancer and antiarthritic drugs. **13 hrs**

Module 3

Metalloproteins

Transport and storage of dioxygen: Heme proteins and oxygen uptake, structure and functions of haemoglobin and myoglobin, dioxygen binding, model complexes; Nonporphyrin systems-hemerythrin and hemocyanin.

Structure and functions of metalloproteins in electron transfer proteins-cytochromes, ferredoxins and rubredoxins. **8 hrs**

Module 4

Metalloenzymes

Zinc enzyme – carboxypeptidase, carbonic anhydrase and alcohol dehydrogenase.

Copper enzyme- superoxide dismutase.

Molybdenum enzyme- oxotransferase enzyme, xanthineoxidase.

Iron enzyme- catalase, peroxidase and cytochromeP-450.

Coenzymes containing cobalt, vitamin B_{12}, Co-C bond cleavage, mutase activity of coenzyme B_{12}, alkylation reactions of methyl cobalamin. **7 hrs**

Photosynthesis and nitrogen fixation

Nitrogen fixation; Nitrogenase-bacterial nitrogenase systems and synthetic studies. Phtotosynthesis: Chlorophyll, PS I & PS II in cleavage of water. **4 hrs**

SUGGESTED BOOKS

1.Inorganic and Organometallic reaction mechanisms, J.D.Atwood, Brooks/cole publishing co. (1985).

2.Reaction mechanisms of Inorganic and Organometallic systems, J.B. Jordon, Oxford University press, 2nd edition (1998).

3. Inorganic Chemistry, G.L Miessler and D.A. Tarr,

4. Modern Inorganic chemistry , W.L.Jolly, 2nd edition McGraw –Hill, Inc.

5. Principles and Application of Organotransition metal chemistry, J.P.Collmanm, L.S. Hegedus, J.R. M.Norton and R.G. Finke, University Science Books, (1987).

6. Inorganic Chemistry, G. Wulfsberg, Viva Books private Ltd. (2002).

7. Bioinorganic chemistry, K.Hussain Reddy.New Age international publishers(2003).
8. Bio-inorganic chemistry, I.Bertini, H.B.Gray, S.J.Lippard & J.S.Valentine, Viva Books Pvt. Ltd.(1998).
9. Principles of Bioinorganic Chemistry, S.J. Lippard and J.M.Berg,Panima Pub Corporation (1997).

MSCCH 302

Organic chemistry

55 hrs

Molecular rearrangements, Heterocyclic chemistry and chemistry of natural products

Module 1

Molecular rearrangements: Introduction

Carbon to carbon migration: Pinacol-pinacolone, Wagner-Meerwein, Benzidine, Demjanov, benzylic acid, Favorskii, Arndt-Eistert synthesis, Fries rearrangement, Steven's rearrangement, dienophine rearrangement

Carbon to nitrogen migration: Hofmann, Curtius, Lossen, Schmidt and Beckmann rearrangements.

Miscellaneous rearrangements: Sommelet-Hauser, Wittig, Smiles, Neber, Japp-Klingemann rearrangement, Meisenheimer rearrangements, Bayer-Villeger rearrangement, Allylic rearrangements.

Retrosynthesis: Introduction to disconnection approach: Basic principles and terminologies used in disconnection approach. One group C-X and two group C-X disconnections. Synthons and synthetic equivalents.

Retrosynthesis and synthesis of benzofurans, *p*-methoxy acetophenone, saccharine, α-bisabolene, nuciferal, tetralone, iboprofin. **20 hrs**

Heterocyclic chemistry: Nomenclature of heterocyclic systems; Structure, reactivity, synthesis and reactions of furan, pyrrole, thiophene, indole, pyridine, quinoline, isoquinoline, pyrazole, imidazole, pyrone, coumarin, chromones, pyrimidines and purines. Synthesis and synthetic applications of azirines and aziridines, isoxazole and azepine.

Module 2

Amino Acids: General structure, Physiological properties

Peptides: Structure and conformation of peptide bond, peptide synthesis: Solution phase and Merrifield's solid phase synthesis, Racemization and use of HOBt, Synthesis of

oxytocin and vasopressin, biological importance of insulin, selective cleavage of polypeptide bonds (chemical and enzymatic).

Proteins: Structure determination: *C* and *N* terminal residue determination, primary, secondary, tertiary and quartenary structure determination, denaturing and renaturing of proteins.

Nucleic acids: Introduction, structure and synthesis of nucleosides and nucleotides, Solid phase synthesis of oligonucleotides, Structure of RNA and DNA, Crick-Watson model, role of nucleic acids in the biosynthesis of proteins. **18 hrs**

References:

1. J. March, Advanced Organic Chemistry, Wiley Inter Science, 1994.
2. F.A. Carey and Sundberg, Advanced Organic Chemistry – Part A & B, 3rd edition, Plenum Press, New York, 1990.
3. Principles of Organic Synthesis ROC Norman and Coxon.
4. Comprehensive Organic Synthesis – B.M. Trost and I. Fleming series, Pergamon Press, New York, 1991.
5. S.K. Ghosh, Advanced General Organic Chemistry, Book and Allied (P) Ltd., 1998.
6. Heterocyclic Chemistry – Joule & Smith
7. Basic Principles of Heterocyclic Chemistry – L.A. Pacquette
8. Molecular reactions and Photochemistry-DePey Chapmann
9. Organic synthesis- Stuart Warren, Wiley interscience, 1982.

MSCCH 303

Physical Chemistry

55 hrs

Module 1

Quantum Mechanics

Part A

Introduction and objectives; Wave- particle duality, Bohr theory of hydrogen atom, Sommerfeld theory. Progressive and stationary waves, matter waves of de-Broglie; Classical wave theory, Heisenberg uncertainty principle. Eigen functions and Eigen values, Co-ordinate transformations, Operators, shifting of classical to quantum mechanical wave function, linerar and angular momentum operators, development of Schrödinger equation, Time-dependent and independent, relations, interpretation of ψ, normalization and orthoglonalization of wave function. Class Q functions, Commutation relations; Postulates of quantum mechanics, Hermitian operator, theorems concerning hermitian operators, Stationary states in quantum mechanics. Solutions of Schrödinger equation for a free particle, particle on a ring and particle in 3-D. **8hrs**

Part B

Application of Schrödinger equation to harmonic oscillator and rigid rotator. Ladder operator method for angular momentum. Schrödinger equation to hydrogen atom in spherical polar coordinates. Solution of Φ, Θ equations and statement of solution of R equation. Total wave function of hydrogen atom. Diagrams of radial and angular wave functions. Radial and angular distribution functions and their significance. Electron spin (Stern-Gerlach experiment), spin orbital, anti-symmetry and Pauli exclusion principle, Slater determinants. Coupling of angular momenta. Russell-Saunders and JJ-coupling, Term symbols. Zeeman Effect. Slater Orbitals ENC for 1s, 2s, 3s, 2p and 3d electrons.

7 hrs

Part C

Approximate methods: Need for approximate methods. Perturbation method. Rayleigh Schrödinger Perturbation theory for time-independent non-degenerate system. Application to electron in a box under the influence of an electric field. Application to

He atom. Variation theorem-Statement and proof. Application of variation method to He atom multi electron system, particle in 1-D box, linear oscillator, calculation, SCF method for many electron atoms. HMO theory for conjugated systems. Application to ethylene, ally radical, butadiene and benzene, Electronic energy states of H-atom. Degeneracy, Wave equation for H-atom, separation and solution of R, ϕ and θ equations. Review of rigid rotor, harmonic oscillator and H- atom problems. Radiative transitions.

8 hrs

Module 2

Chemical Thermodynamics

A brief resume of laws of thermodynamics (combined form of 1^{st} and 2^{nd} laws), entropy as a measure of unavailable energy, Concept of fugacity and free energy, entropy and free energy changes and spontaneity of processes. Variation of free energy with T & P, Maxwell's relations, thermodynamics equations of state, limitations of Van't Hoff`s equation, Nernst heat theorem & its applications.Third law of thermodynamics, determination.of third law of entropies **6hrs**

Application of thermodynamics

Entropy and free energy of mixing, partial molar quantities, partial molar volume and free energy (chemical potential), their significance and determinations. Gibbs-Duhem and Duham-Margules equations.

Partial molar volumes , their significance and their determination by intercept method and from density measurements. Chemical potential and its significance. Variation of chemical potential with temperature and pressure. Formulation of the Gibbs Duhem equation. Derivation of Duhem-Margules equation. Raoult's law, Henry's law. Ideal and non-ideal solutions.

Partial molar properties- partial molar free energy, partial molar volume, partial molar heat content and their significance. Determination of these quantities. **5 hrs**

Module 3

Fast Reactions

Kinetics of fast reaction; Steady state approximation and simple examples relating kinetics to mechanism. Study of kinetics by flow techniques, equation for contact time, stopped flow and continuous flow methods. Relaxation method, equation for relaxation

time, temperature jump and pressure jump methods, flash photolysis. NMR method. Theories of unimolecular reactions, Perrin theory, Lindemanntheory, Hinshelwood theory, RRKM theory, Slater treatment. **5hrs**

Fugacity

Determination of fugacity of gases. Variation of fugacity with temperature and pressure. Activity and activity coefficients. Variation of activity with temperature and pressure. Determination of activity coefficients by vapour pressure, Fugacity of real gases, Determination of fugacity of real gases using graphical method and from equation of state. Equilibrium constant for real gases in terms of fugacity. Gibbs energy of mixing, entropy and enthalpy of mixing. **4hrs**

Module 4

Symmetry and Group Theory

Definitions of group, subgroup, relation between orders of a finite group and its subgroup.

Symmetry elements, Symmetry operations and point group. definition of a point group, classification of molecules into point groups. Mulliken symbols. Geometries of metal complexes of higher coordination numbers. Determination of point group. Construction of group multiplication tables. Symmetry species and character tables. Reducible and irreducible representations. Analysis of reducible representations. Number of normal modes of vibrational symmetry types. Rule of mutual exclusion. I.R.and Raman active fundamentals.

Conjugacy relation and classes, symmetry elements and symmetry operations, Schonflies symbols, Matrix representations of symmetry operations, products of symmetry operations, some properties of matrices and vectors, classification of molecules into point groups. The Great Orthogonality theorem (without proof), character tables. The direct product. Applications of group theory - Molecular vibrations, group theoretical selection rules for electronic transitions, for IR and Raman spectra. **12 hrs**

SUGGESTED BOOKS

1. Physical Chemistry, P.W.Atkins, Julio de Paula, ELBS, 7th edition, (2002).
2. Physical Chemistry: A Molecular Approach, McQuarie and Simon, Viva, New Delhi (2001).
3. Introduction to Quantum Chemistry, A.K.Chandra, Tata McGraw Hill, (1988)
4. Quantum Chemistry, Ira N.Levine, Prentice Hall, New Jersey, (1991)
5. Coulson's valence, R.Mc Weeny, ELBS, (1982).
6. Quantum Chemistry, 2nd edition, R. K. Prasad, New Age International,(2000).
7. Quantum Chemistrry Through Problems and Solutions, R. K. Prasad, New Age International (1997).
8. Chemical Kinetics-K.J.Laidler, McGraw hill. Inc. New York (1988).
9. Principles of Chemical Kinetics-House J.E. Wm C Brown Publisher, Boston, (1997).
10. Kinetics and Mechanism- A.A. Frost and R.G.Pearson , John-Wiley, New York, (1961).
11. Chemical kinetics Methods-C.Kalidas, New Age International Publisher, New Delhi (1995)
12. Kinetics of Chemical Reactions-S.K.Jain Vishal Publications, Delhi (1982).
13. Kinetics and Mechanism of Chemical Transformation-J.Rajaraman and J.Kuriakose, Mc Millan. (1986).
14. Chemical Applications of Group Theory, F. A. Cotton, Wiley Eastern (1976).
15. Molecular Symmetry, D. S. Schonland, Van Nostrand (1965).

MSCCH 304

Analytical Chemistry-I

55 hrs

Module 1

Data analysis

Introduction to analytical chemistry, classification of analytical methods, Factors affecting the choice of analytical method. Limitations of analytical methods – Error: determinate and indeterminate errors, minimization of errors. Accuracy and precision, distribution of random errors, the normal error curve. Statistical treatment of finite samples - measures of central tendency and variability: Mean median, range, standard deviation and variance. Comparison of results - student's t-test, F-test. Significant figures, confidence intervals, method of least squares, calibration curves and standard addition method. Figures of merit of analytical methods - sensitivity and detection limit, linear dynamic range.

11 Hrs

Module 2

Separation techniques I

Chromatography: Definition, principles and mechanism of separation, classification of chromatographic techniques. General descriptions of column chromatography - frontal analysis, displacement analysis and elution analysis. General theory of column chromatography: characterizing a chromatogram - retention time, retention volume and

baseline width. Chromatographic resolution, capacity factor, column selectivity. Column efficiency - band broadening - rate theory and plate theory. Peak capacity, non ideal behavior. Optimizing chromatographic separations using capacity factor, column selectivity and column efficiency - Van Deemter equation, and its modern versions, Golay equation and Huber-Knox equations.

Thin layer chromatography: Principle, apparatus and methodology, applications.

Gas chromatography (GC): Principles, instrumentation **-** mobile phase, chromatographic columns, stationary phases, sample introduction, temperature control, and detectors for gas chromatography. Quantitative and qualitative applications.

High performance liquid chromatography (HPLC): Principles, instrumentation - columns (analytical and guard columns), stationary phases, mobile phases, choosing a mobile phase, isocratic *vs* gradient elution, HPLC plumbing, sample introduction. Detectors for HPLC - spectroscopic, electrochemical and others, quantitative applications. 16 Hrs

Module 3

Separation techniques II

Supercritical fluid chromatography (SFC): Properties of supercritical fluids, instrumentation and operating variables, comparison of SFC with other types of chromatography, applications.

Solvent Extraction: Types-batch, continous, efficiency, selectivity, Distribution coefficient, Nernst distribution law, derivation, applications and numerical problems.

Electrophoretic methods: Electrophoresis & Capillary Electrophoresis**:** Theory **-** electrophoretic mobility, electroosmotic mobility, electroosmotic flow velocity, total mobility, migration time, efficiency, selectivity and resolution. 8 Hrs

Module 4

Thermal methods of analysis

Thermobalance, Factors influencing thermogravimetric results, Differncial thermal analysis- Instrumentation for differential thermal analysis (DTA), and differential scanning calorimetry (DSC). Applications of TG, DTA and DSC. 7 hrs

Optical Methods of chemical analysis

Interaction of electromagnetic radiation with matter, Beer-Lambert's law, derivation, verification, deviations, molar extinction coefficient, choice of solvent, Sandell sensitivity, Ringboms' plot, photometric titrations, Single beam & double beam UV-VIS spectrophotometer, Application of quantitative and qualitative analysis, Principle, Instrumentation and applications of Fluorimetry. Numerical problems on all these techniques. 9 hrs

Radioanalytical Methods

Radioactivity, Ionisation, Working principles of GM counter, γ-ray counter, neutron activation analysis, Isotopic dilution analysis, Radiotracer technique, Applications of all these techniques, Use of radioactive isotopes in solving analytical and Physico chemical problems. 4 hrs

SUGGESTED BOOKS

1. Fundamentals of Analytical Chemistry, Eighth Edition, Skoog,West,Holler and Crouch; Thomson Asia Pvt. Ltd
2. Analytical Chemistry. G. D. Christian, V Edition, John – Wiley and Sons Inc.,

3. Instrumental methods of Chemical Analysis, G. W. Ewing, 5th edition, McGraw-Hill, New York, 1988.
4. Vogel's text book of Quantitative Chemical analysis 5th edition, Ed., Jeffery et. al ELBS/Longman, 1989
5. Instrumental methods of Analysis. H. H. Willard, L. L. Merit , J. A. Dean and F. A. Set, CBS Publishers (1996).

MSCCH 305

Physical Chemistry Practical – II

1. Study of kinetics of photo degradation of Indigo carmine using TiO_2 as photo catalyst.

2. Determination of the molecular weight of a polymer material by viscosity measurements (cellulose acetate/methyl acrylate).

3. Study of decomposition of diacetone alcohol using dilatometer - Evaluation of catalytic coefficient of OH^- ions, Ea and thermodynamic parameters.

4. Determination of solubility and solubility product of sparingly soluble salt conductometrically.

5. Conductometric titration of KCl with AgNO3

6. Determination of redox potential of Fe2+ ions by potentiometric method.

7. Potentiometric titration of Pb(NO3)2 Vs EDTA.

8. Potentiometric titration of KI vs KMnO4 solution.

9 Construction of Phase diagram of a two-component system and determination of eutectic temperature and eutectic composition.

10 Determine the Critical Solution Temperature of Phenol-water system.

11. Construct the phase diagram of the three component of partially immiscible liquid system (DMSO-water-benzene; acetone-chloroform -water; chloroform-acetic acid water)

12. Determination of partial molar volume of (a) NaCl-H2O systems.

13. Distribution coefficient of I2 between two immiscible solvents.

14. Study the inversion of cane sugar in the presence of acid using Polarimeter

15. Spectrophotometric analysis of a mixture of (a) CuSO4 and K2CrO4.

16. Study of the redox behaviour of $K_4Fe(CN)_6$ / $K_3Fe(CN)_6$ using cyclic voltametry

17. Estimation of a metal ion in solution by polarographic method.

18. Amperometric titration of lead nitrate against potassium chromate/potassium dichromate.

19. Adsorption of acetic acid on charcoal to verify Freundlich adsorption isotherm.

20. Determination of molecular weight of a compound using Bekmann's cryoscopic method using benzene or/and water as solvent.

21.Titration curve of amino acid with acids and bases

22. Determination of iodine value of Lipids

SUGGESTED BOOKS

1. Findlay's Practical Physical Chemistry revised by Levitt, Longman's London (1966).
2. Experiments in Physical Chemistry by Shoemaker and Garland, McGraw Hill International edn.(1996).
3. Advanced Practical Chemistry by J.B. Yadav, Goel Publication house, Meerut(1989).
4. Experimental Physical Chemistry by Daniel etal., McGraw Hill (1962).
5. Experimental Physical Chemistry by Wilson, Newcombe and others, Pergamon Press, New York (1962).
6. Practical Physical Chemistry by A,M. James and D.E. Pritchard, Longman Group Ltd. (1968).
7. Experimental Physical Chemistry, V. D. Athawale and Parul mathur, New Age International, New Delhi (2001).
8. Experiments in Physical Chemistry, J. G. Ghosh , Bharathi Bhavan, (1974).

MSCCH 306

Inorganic Chemistry practicals –III

(4 days a week 4 ½ hours a day)

1. Gravimetric determination of Haematite ore.
2. Gravimetric determination of Pyrolusite ore.
3. Complexometric determination of Copper and Manganese.
4. Volumetric and gravimetric determination of Copper and Nickel
5. Volumetric and gravimetric determination of Copper and Iron.

6. Volumetric and gravimetric determination of Copper and Zinc.
7. Volumetric and gravimetric determination of Nickel and Zinc.
8. Colorimetric determination of Nickel.
9. Colorimetric determination of Iron.
10. Preparation and analysis of Potassium tris(oxalato)ferrate(III)trihydrate.
11. Preparation and analysis of cis and trans potassium dioxalatodiaquochromium(III) complex.
12. Preparation of potassium tris(oxalato)aluminate(III)trihydrate.
13. Preparation of pentamminechlorocobalt(III)chloride.
14. Preparation and IR spectral studies of Pentamminenitrocobalt(III) chloride and the corresponding nitrite complex.
15. Paper chromatographic separation of Co^{2+},Ni^{2+} and Cu^{2+} ions.
16. Separation of Biomolecules by TLC .
17. Fluoremetric analysis of DNA damage.

SUGGESTED BOOKS

1. Vogel's Text book of Qualitative Chemical Analysis, J.Bassett, G.H. Jeffery and J.Mendham, ELBS (1986).
2. Vogel's Text book of Quantitative Chemical Analysis, 5th Edition,J.Bassett, G.H. Jeffery and J.Mendham,and R.C.Denny, Longman Scientific and Technical (1999).
3. Inorganic Semimicro Qualitativwe Analysis, V.V. Ramanujam, The National Pub.Co.(1974).
4. Practical Inorganic Chemistry, G.Marr and B.W. Rockett, Von Nostrand Reinhold (1972).

Semester IV

MSCCH 401

Analytical Chemistry - II

55 hrs

Module 1

Titrimetric Analysis

Acid – Base Titrations: Basic principles, Titration curves for mono functional acids and bases, pH calculations, theory of indicators, fractions of phosphoric acid species as a function of pH. Titration curves for polyfunctional acids [H_3PO_4], polyamines and amino acid systems. **5 hrs**

Redox Titrations: Nernst equation, Standard & formal potentials. Titration curves, end point signals, Indicators, criteria for the selection of indicators. Feasibility of redox titration. Titration of multicomponent system. Adjustment of analyte's oxidation state. Applications: Oxidants such as Permanganate, dichromate, Ce (IV), bromate, Iodates.

6 hrs

Precipitation titrations: Solubility product. Theoretical principles: Titration curves, end point signals, Mohr, Volhard and adsorption indicators. Applications: Estimation of F^-, K^+, CO_3^{2-}, $C_2O_4^{2-}$, acetylenes and mixture of halides. **4 hrs**

Complexometric titrations: Complexometric titrations with particular reference to EDTA titrations, suitability of polydentate ligands as titrants, expressions for the different forms of EDTA in solution as a function of pH, conditional stability constants, derivation of titration curve, effect of pH and second complexing agent on the conditional stability

constant and titration curve. Selectivity by pH control, masking and demasking, metal ion indicators, types of EDTA titrations, titrations involving monodentate ligands

6 hrs

Module 2

Electroanalytical techniques

Electrode Potentials, Currents in Electrochemical cells, Potentiometric titrations. Electrogravimetry, Coulometry, and Coulometric titrations. Amperometry

Voltammetry at a dropping mercury electrode (DME): Review of the principles of normal dc polarography – types of currents obtained at a DME – Ilkovic equation and its application – current-potential relation for a cathodic process – half-wave potential – tests for the reversibility of a process – irreversible processes at a DME – factors that set the sensitivity and selectivity limits in normal dc polarography.

Modified polarographic techniques: Tast polarography – normal pulse polarography – differential pulse polarography – ac polarography.

Stripping analysis: Hanging drop mercury electrode (HDME) – principle and applications of cathodic and anodic stripping voltammetry.

Cyclic voltammetry: Principle – experimental set up – quantitative analysis – determination of diffusion coefficients – diagnostic criteria for reversible, quasi-reversible and irreversible processes – study of coupled chemical reactions like E_rC_r, C_rE_r and $E_rC_iE_r$.

Chronomethods: Basic concepts, methodology and applications of chronoamperometry, chronocoulometry and chronopotentiometry.

Spectroelectrochemical techniques: Principle and application of transmission IR spectroelectrochemical technique.

Hydrodynamic electrodes: Construction and use of rotating disc and rotating ring disc electrodes in the study of electrochemical processes. **15 hrs**

Module 3

Sampling and preparing samples for analysis

Importance of sampling, designing a sample plan-random, judgement, systematic-judgement, stratified and convenience sampling. Type of sample to collect-grab and composite samples. Insitu sampling. Size of sample and number of samples. Implementing the sampling plan-solutions, gases and solids. Bringing solid samples into solution-digestion and decomposing. **5 hrs**

Soil Analysis

Physical properties of soils - soil texture and soil structure. Chemical properties of soil-types of soil colloids, types of clays and their swelling and adsorption properties, cation exchange capacity and its determination, acid soils-types of soil acidity, liming, measurement of pH and conductivity of soil- saline and alkaline soils, analysis of major constituents of soil-organic matter, nitrogen, sulphur, sodium, potassium and calcium.
5 hrs

Module 4

Analysis of Drugs and Poisons

Classification of drugs; Characterisation of common drugs: Analgesics-aspirin, paracetamol, Expectorants- Benadryl, Vitamins- A and C, Sedatives- diazepam, barbiturates, Antibiotics- penicillin, chloramphenicol, ampicillin,Cardiovascular-sorbitrate, methyldopa. Drugs of abuse: Analysis of narcotics (nicotine, morphine, heroin) and other dangerous drugs; screening by gas and thin-layer chromatography and

spectrophotometric measurement, Estimation of drug residues in biological samples. General discussion of poisons with special reference to mode of action of snake venom, war gases, cyanide, carbon monoxide and opium. Estimation of cyanide, carbon monoxide and barbiturates. **8 hrs**

SUGGESTED BOOKS

1) Fundamentals Of Analytical Chemistry-Skoog, West And Holler 7th Edition Saunders College Publishing Int.Ltd. (1996)

2) Modern methods of Chemical analysis-Pecsok, Shields, Cairns and McWilliams (2nd edition), John Wiley and Sons (1976).

3) Vogel's Textbook of Quantitative Inorganic Analysis, Bassett, Denney, Jeffery and Mendham, (4th edition) ELBS (1989).

4) Analytical Chemistry-G.D.Christian (5th edition) John Wiley & sons (19946).

5) Treatise on analytical Chemistry-Kolthoff, Elving and Krivan (2nd edition) John Wiley & Sons (1986).

6) Methods of Soil Analysis Part I & II, C.A. Black et al (Ed) American Society of Agronomy, Inc. (1965)

7) A text book of Soil Chemical Analysis – P.R. Hesse, CBS Publishers, (1994).

MSCCH 402

Spectroscopy-II

55 hrs

Module 1

IR Spectroscopy

Characteristic group frequencies and skeletal frequencies. Finger print region, Identification of functional groups- Alkenes, Aromatics, Cabonyl compounds (aldehydes and ketones, esters and lactones), halogen compounds, sulphur and phosphorus compounds, amides, lactums amino acids and amines. Factors affecting group frequencies and band shapes, conjugation, resonance and inductance, hydrogen bonding and ring strain. Tautomerism, Cis-trans isomerism. Characteristic vibrational frequencies

of alkanes, alkenes, alkynes, aromatic compounds, alcohols, ethers, phenols, amines; Detailed study of vibrational frequencies of carbonyl compounds (ketones, aldehydes, esters, amides, acid anydrides, lactones, lactams, conjugated carbonyl compounds); Effects of H-bonding and solvent effect on vibrational frequency, extension to various organic molecules for structural assignment. Effects of H-bonding and solvent effecton vibrational frequency, extension to various organic molecules for structural assignment. Infrared spectra of simple molecules and coordination compounds, changes in infrared spectra of donor molecules upon coordination (N,N-dimethylacetamide, urea, DMSO, pyridine N-oxide, ammine, cyano, cyanato and thiocyanato complexes), mono and multinuclear carbonyl complexes, nitosyls, phosphine and arsine complexes. Change in spectra accompanying change in symmetry upon coordination (NO3-, SO42-, NO2-, and ClO4), hydrogen bonding. **10 hrs**

Ultraviolet spectroscopy

Factors affecting the position and intensity of UV bands – effect of conjugation, steric factor, pH, solvent polarity, types of transitions, effect of substituents. Calculation of absorption maxima by Woodward-Fieser Rules (using Woodward-Fieser tables for values for substituents) for the following classes of organic compounds: conjugated polyenes (cyclic and acyclic), enones and substituted benzene derivatives. Theory of molecular absorption. Vibration rotation fine structure of electronic spectra. Types of absorption bands: C-T & ligand field. Empherical rules for predicting the wavelength of maximum absorption: Olefins, conjugated dienes, cyclic trienes and polyenes unsaturated aldehydes and ketones-benzene and substituted benzene rings. Basic components of instrumentation, singleand double beam designs. Applications: Qualitative and quantitative analysis of binary mixtures, measurement of dissociation constants of acids and bases, determination of molecular weight, photometric titrations, determination of stoichiometry and stability of the complexes and kinetic studies. **8 hrs**

Module 2

Electronic absorption Spectroscopy

Term symbols, energies of atomic and Molecular transitions, Selection rule, Morse potential energy diagram, electronic transitions, polarized absorption spectra. Nature of absorption spectra, nature of absorption spectra of transition metal complexes, Orgel diagram, Tanabe Sugano diagram, charge transfer spectra. **5 hrs**

Electron spin resonance spectroscopy

ESR of d1 and d9 transition metal ions in cubic and tetragonal ligand fields; evaluation of g values and metal hyperfine coupling constants. Basic principles, factors affecting g values, hyperfine coupling, spin densities and McConnell relationship. Zero field splitting. Theortical principles and instrumentation. ESR spectra of hydrogen and nitrogen atoms, Semi-quinone ion, napthalene negative ion, methyl radical and methyl substituted radicals. Zero field splitting, Kramer's degeneracy. Measurements of distribution of unpaired electrons in radicals. Study of co-ordination compounds by ESR technique. **10 hrs**

Module 3

Nuclear Quadrupole Resonance Spectroscopy

Quadrupole nuclei, Quadrapole movement, The NQR experiment, Theory and instrumentation. Effect of magnetic field on the spectra, relationship between electric field gradients, q and molecular structure. Applications. The interpretation of eQq. Data effect of crystal latties on the magnitude of eQq Structural information from NQR spectra. **5 hrs**

Mossbauer Spectroscopy

Introduction, Principles, conditions for Mössbauer spectroscopy, parameters fromMossbauer spectra, isomer shifts, electric quadrupole interaction, magnetic interactions,Mossbauer spectrometer, applications, Fe3(CO)12, Prussion blue, Oxyhemerythrin,Hexacyanoferrates, Nitropruside, Tin halides and $I_2Br_2Cl_4$. **5 hrs**

Module 4

Photoelectron spectroscopy

Basic principles; Photo-electric effect. Ionisation process, Koopman's theorem. Photoelectron spectra of simple molecules, ESCA, chemical information from ESCA. Instrumentation. Auger electron spectroscopy, basic ideas. B] Instrumentation and applications of following techniques photoacoustic Spectroscopy (PAS) photo electron Spectroscopy (PES), auger electron Spectroscopy (AES). **10 hrs**

X-ray spectroscopy

Principles, instrumentation and applications of X-ray fluorescence, absorption and diffraction spectroscopy**.** **1 hrs**

Electron Spectroscopy

Theory, Instrumentation and applications of Scanning electron microscopy (SEM), Scanning tunnelling microscopy (STM) and Atomic force microscopy (AFM). **1 hrs**

SUGGESTED BOOKS

1. Fundamentals of Molecular Spectroscopy-C. N. Banwell

2. Physical Methods in Chemistry-R .S. Drago, Saunder college

3. Structural Methods in Inorganic Chemistry-E. A. Ebsworth, D. W. H. Ranbin and S. Cradock, ELBS

4. Infrared Spectra of Inorganic and Coordination Compounds, K. Nakamoto.

5. Infrared Spectroscopy-C.N.R. Rao.

6. Electron Absorption Spectroscopy and Selected Techniques-D. N. Satyanarayana, University Prof. India Ltd. Hyderabad.

7. Introduction to Spectroscopy-Pavia, Lampman and Kriz

8. P.R. Backer: Molecular symmetry and Spectroscopy A.P.
9. Ferraro Ziomeek, Introduction to Group theory, plenum
10. CNR Rao Spectroscopy in Inorganic Chemistry Vol I,II,III
11. Chemical Application of Mossbaur Spectroscopy, Goldanski V.I & Harber R.H., Academic Press 1968.

MSCCH 403

Bio Chemistry

55 hrs

Module 1

Basic Concepts & Introduction to Biomolecules

Introduction to Biochemistry, types of chemical reactions, pH, buffers &their properties, concentration of solutions.

Carbohydrates: Types, classification, properties, structures. Fats and lipids: Definition, types, classification, properties, structures, phospholipids, glycolipids, steroids. Amino acids and proteins: Definition, types, classification, properties, structures. Peptides with few examples. Nucleic acids: Definition, types, purines, Pyrimidines, DNA & RNA.

11 hrs

Module 2

Principles of Bioenergetic

Energy, energy flow cycle, energy conversion, structure & properties of ATP.Coupling reactions of ATP &NDP. Concepts of thermodynamics. Photosynthesis: Chloroplasts, light reactions & dark reactions.

Introduction to enzymes: Definition, types, classification, models proposed to explain E-S complex, enzyme kinetics, and inhibition.

Electron transport chain and oxidative phosphorylation: Energetics, Energy balance sheet, oxidative stress.

11 hrs

Carbohydrate Metabolism

Glycolysis- Metabolism, aerobic and anaerobic pathway, its regulation, TCA cycle, Calvin cycle, Glyoxylate cycle, PP pathway, gluconeogenesis, & its regulation. Biosynthesis & degradation of polysaccharides (glycogen). **6 hrs**

Module 3

Lipid Metabolism

Biosynthesis of fatty acids, cholesterol, phospholipids, glycolipids, biodegradation of fatty acids.

5 hrs

Aminoacid Metabolism

Biosynthesis of aminoacid starting from acetyl coA (with reference to Oxaloacetate family). Biodegradation of amino acids, deamination, transamination & urea cycle.

4 hrs

Nucleic acid Metabolism

Biosynthesis, biodegradation and regulation of Purines, Pyrimidines and nucleic acids.

5 hrs

Module 4

Membrane Biochemistry

Structure, permeability, properties,types of transport, facilitated transport, passive transport, active transport, energy requirement. Mechanism of Na^+ K^+ ATPase, glucose and aminoacid transport. Action potential &signal transduction. **5 hrs**

Metabolic disorders

Inborn errors of metabolism, disorders of carbohydrate, lipid and aminoacid metabolism. Hormonal imbalances, vitamins, minerals and micronutrient deficiencies. **5 hrs**

SUGGESTED BOOKS

1. Nelson & Cox., Lehninger's Principles of Biochemistry.
2. Harper, Harper's Illustrated Biochemistry
3. Stryer, Biochemistry.
4. Hermann Dugas, Bioorganic Chemistry.

MSCCH 404

Industrial Chemistry

55 hrs

Module 1

Chemometrics:

Stoichiometry of chemical reactions, concept of kgmol, limiting reactant, theoretical and practical yield. Concentration of a solution based on volume and mass units. Solubility and solubility equilibria, effect of presence of common ion. Calculations of pH of acids, bases and acidic and basic buffers. Concept of formation constants, stability and instability constants, step wise formation Constants**.**

10 hrs

Module 2

Unit Processes In Organic Synthesis:

1. **Nitration** :

Introduction, Nitrating Agents, Aromatic Nitration, Kinetics & Mechanism of Aromatic Nitration, Nitration of Paraffinic hydrocarbons, Nitrate Esters, N-NitroCompounds, Process Equipment for Technical Nitration, Batch Nitration, Continuous Nitration, Mixed acid compositions, DVS calculations, Typical Industrial Nitration Process- Preparation of Nitrobenzene, Preparation of mdinitrobenzene

3. Halogenation :

Introduction, Chlorination, Bromination, Fluorination, Iodination.

4. Sulfonation & Sulfation :

Introduction, Sulfonating & Sulfating agents, Sulfonation of Aromatic compounds, Benzene & its derivatives, Naphalene & its derivatives, Anthraquinone & its derivatives.

Unit Process in Inorganic synthesis :

1. Industrial Process of Sulfur & Sulfuric acid

2. Nitrogen Industries : Ammonia, Nitric acid & Urea

3. Ore processing: Ore processing/ Beneficiation: Definition of ore. Types of ores, operating steps involved in ore processing / dressing / beneficiation: coominution, sizing and screening, concentration and filter processing.

Different process of concentration of ore minerals, Beneficiation of Pb-Zn-Cu ore iron ore, Zn ore etc. Beach sands and graphite, leaching as a means of ore processing.

25 hrs

Module 3

Plant Utilities

1. Water

Sources of Water, Hard & Soft water, Causes of Hardness, Disadvantages of hard water, Methods of softening of water, Preboiling of water-Lime soda Process-Ion Exchange process. Essential characteristic of drinking water, purification of water-Screening, Sedimentation, Coagulation, Filteration, Treatment to Boiler Feed Water-Formation of Scale, Corrosion, Priming & Foaming, Caustic embrittlement.

2. Insulation

Introduction, Insulating Factors, properties of good insulator, Classification-Glass Wool Properties & application, Cold Insulation, Low Temperature Insulation.

3. Steam & Steam Generator

Steam-Formation of Steam at constant Pressure, Enthalpy-Enthalpy of water, Enthalpy of Evaporation, Enthalpy of dry saturated steam, Wet Steam, Superheated Steam, Specific Volume of steam. Steam Generator- Classification, Factors for Boiler selection

4. Air Compressed air, Fan air Reciprocating Air Compressors, Multistage Compressors.

10 hrs

Module 4

Industrial Safety:

1. **Introduction: -** Definition & terms used in context of safety, Accident- Nonreportable

accidents. Hazard, Risk, Acceptance Physical factors for Accidents- Accident ratio, Safety Training, Role of Supervisor in achieving a high standard of Safety, Supervisory Training, Motivation for safety-Safety Suggestion Scheme, Safety Committee, Safety Competition-Safety Contests, Safety Drives, Safety Exhibition & Poster.

2. **Fire & Explosion :-** The Chemistry of Fire, Fire triangle, Classification of Fire, Stages of Fire, Causes of Industrial Fire-Electrical Equipment, Smoking, Mechanical Fault, Welding & Gas Cutting, Sparks, Explosives Dusts, Static spark, Runaway Chemical Reaction, Fire Extinguishers-Fixed Fire fighting system. Portable fire Extinguishers-Soda acid type, Dry Chemical Powder type, Carbon dioxide type & Foam type Extinguisher.

3. **Personal Protective Equipment: -** Hand Protection, Foot Protection, Head Protection, Eye Protection, Face Protection, Skin & Body Protection, Protection against Fall, Noise Protection, Respiratory Protection-Care & Precaution, External air supply type & Self-Contained Breathing apparatus (SCBA), Selection of Personal protective equipment.

10 hrs

MSCCH 405

Nanotechnology

55h

Module 1

Introduction to Nono

Nano and nature, basic nanostructures , nanocomposites, Thin films, nanofoam, nanoclusters **3 hrs**

Size Effects in Nanochemistry

Models of Reactions of Metal Atoms in Matrices, Melting Point, Optical Spectra, Kinetic Peculiarities of Chemical Processes on the Surface of Nanoparticles, Thermodynamic Features of Nanoparticles **5 hrs**

Synthesis of nanomaterials

Physical Methods: Inert gas condensation, Arc discharge, RF-plasma, Plasma arc technique, Ion sputtering, Laser ablation, Laser pyrolysis, Ball Milling, Molecular beam

epitaxy, Chemical Vapour deposition (CVD) method and other variants, Electrodeposition. **10 hrs**

Module 2

Chemical Methods: Solg-gel, , hydrothermal, solvothermal, ionothermal synthesis, combustion method, microwave method, coprecipitation method, Photochemical synthesis, Electrochemical synthesis, Nanocrystals of semiconductors and other materials by arrested precipitation, Thermolysis routes, Sonochemical routes, Liquid-liquid interface, Hybrid methods, Solvated metal atom dispersion, Post-synthetic size-selective processing. Micelles and microemulsions, Cluster compounds. Surfactants, types, ex.

Characterization of

X-ray diffraction, SEM, FESEM, TEM, HRTEM, SAED patterns, EDS analysis, AFM, UV-Visible Spectrophotometers **6 hrs**

Properties of Nanomaterials

Introduction - Electronic Properties of materials & nanomaterials, role of size in nanomaterials.

Confinement and transport in nanostructure, Optical Properties - Photoconductivity, Optical absorption & transmission, Photoluminescence, Fluorescence, Phosphorescence, Electroluminescence. **6 hrs**

Module 3

Carbon Nanotube (CNT) and Its Functionalization

Preparation of Carbon Nanotubes – introduction, types, CVD and other methods of preparation, Functionalization of Carbon Nanotubes, Reactivity of Carbon Nanotubes,

Preparation and Characterization Fullerene and other associated carbon clusters/molecules, Graphene-preparation, characterization and properties **10 hrs**

Semiconductor quantum dots

Introduction, synthesis of quantum dots, electronic structure of nanocrystals, correlation of properties with size, applications **5 hrs**

Module 4

Core shell nanoparticles

Introdcution, types of system, characterization, ptoperties, applications. **5 hrs**

Nanosensors

Introduction, What is a Sensor, Nanosensors, organization for Sensors, Nanosensors Based on Optical Properties, Nanosensors Based on Quantum Size Effects, Electrochemical Sensors, Nanobiosensors **5 hrs**

SUGGESTED BOOKS :

1) Nano, the essentials, understanding nanoscience and nanotechnology- T. Pradeep, Tata McGraw hill publication.

2) Hari Singh Nalwa - Encyclopedia of Nanotechnology.

3) Introduction to Nanotechnology - Charles P. Poole Jr. and Franks. J. Qwens

4) Nanomaterials Handbook- Yury Gogotsi

5) Springer Handbook of Nanotechnology - Bharat Bhusan

6) Chemistry of Nanomaterials : Synthesis, properties and applications by CNR Rao et.al.

7) Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM **-** Ray F. Egerton

8) Applied Physics Of Carbon Nanotubes : Fundamentals Of Theory, Optics And Transport Devices - S. Subramony & S.V. Rotkins

9) Carbon Nanotubes: Properties and Applications**-** Michael J. O'Connell

10) Carbon nanotechnology- Liming Dai

11) Nanotubes and Nanowires- CNR Rao and A Govindaraj RCS Publishing