



FACULTY OF SCIENCE

DEPARTMENT OF CHEMISTRY

**M. Sc. CHEMISTRY
(CHOICE BASED CREDIT SYSTEM)**

HAND BOOK

2014 – 2015 (Onwards)

**ANNAMALAI UNIVERSITY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
M. Sc. CHEMISTRY
(Choice Based Credit System)**

Regulations and Syllabus (2014 – 2015)

Regulations

Master's Programme

A Master's Programme consists of a number of courses - a set of Core Courses and Optional Course.

The entire course carries credit system. The number and distribution of credits for the courses will be decided by the respective faculties.

A course is divided into two semesters. Odd semester and Even semester.

Credits

The term credit is used to describe the quantum of syllabus for various programs in terms and hours of study. It indicates differential weightage given according to the contents and duration of the courses in the Curriculum design.

The minimum credit requirement for a two year Master's programme shall be **90**.

The core courses shall carry **70** credits and the optional courses shall carry **20** credits.

Courses

Each course may consist of Lectures/ Tutorials/ Laboratory work/ Seminar/ Project work/ Practical training report/ Viva voce etc.

Course Weight

Core and optional courses may carry different weights. For example, a course carrying one credit for lectures will have instruction of one period per week during the semester, if three hours of lecture is necessary in each week for that course then 3 credits will be the weightage. Thus, normally in each of the courses, credits will be assigned on the basis of the lectures / tutorials / laboratory work and other form of learning in a 15 week schedules:

- i. One credit for each lecture period per week.
- ii. One credit for each tutorial per week.
- iii. One credit for each three periods of laboratory or practical work per week.
- iv. One credit for 3 contact hours of project work in a week.
- v. One credit for every two periods of seminar.

Grading System

The term grading system indicates a 10-point scale of evaluation of the performance of students in terms of marks, grade points, letter grade and class.

Course Duration

The duration for completion of a two year Master's programme in any course is four semesters.

Structure of the programme

The Master's programme will consist of:

- i. Core courses which compulsory for all students.

- ii. Optional courses which students can choose from amongst the courses offered by the other department of a faculty as well as by the departments of other faculties. (Arts, Science, Education and Indian Language) or within the Department.
- iii. The Optional subjects will be allotted by counselling by a committee of the respective heads of the Departments under the Chairmanship of the Dean of the Faculty
- iv. Dissertation / Project Work / Practical training / Field work, which can be done in an organization (Government, Industry, Firm, Public Enterprise etc.) approved by the concerned department.

Attendance

Every teaching faculty handling a course shall be responsible for the maintenance of attendance Register for candidates who have registered for the course.

The teacher of the course must intimate the Head of the Department at least seven calendar days before the last instruction day in the semester about the attendance particulars of all students.

Each student should earn 80% attendance in the courses of the particular semester failing which he or she will not be permitted to sit for the End-Semester Examination.

However it shall be open to the authorities to grant exemption to a candidate who has failed to obtain the prescribed 80% attendance for valid reasons on payment of a condonation fee and such exemptions should not under any circumstance be granted for attendance below 70%.

Examinations

The internal assessment for each course theory papers carries 25 % marks and is based on two sectional tests and for practical examination carries 40 % marks and is based on two sectional tests and a variety of assessment tools such as seminar, assignment. The pattern of question paper will be decided by the respective faculty. The tests are compulsory.

For internal assessment evaluation, the break-up marks shall be as follows:

Theory	Internal Marks	Practical	Internal Marks
Test-I	10	Test-I	15
Test-II	10	Test-II	15
Attendance and Assignment	5	Attendance and Record	10
Total	25	Total	40

There will be one End Semester Examination (75% marks for theory and 60 % for practical) of 3 hours duration for each course. The pattern of question paper will be decided by the respective faculty.

Evaluation

The performance of students in each course is evaluated in terms of percentage of marks (PM) with a provision for conversion to Grade point (GP). The sum total performance in each semester will be rated by GPA while the continuous performance from the 2nd semester onwards will be marked by (OGPA).

Marks and Grading

A student cannot repeat the assessment of Sessional Test-I and Sessional Test-II. However, if for any compulsive reason the student could not attend the test, the prerogative of arranging a special test lies with the teacher in consultation with the head of the Department.

A minimum of 50 % marks in each course is prescribed for a pass. A student has to secure 50% minimum in the end semester examination.

If a candidate who has not secured a secured a minimum of 50% marks in a course shall be deemed to have failed in that course.

The student can repeat the End Semester Examination when it is offered next in the subsequent Odd / Even Semesters still the regulations are in force. However, a candidate cannot move to the next odd / even semester if he/she has more than six papers as arrears at any point of time.

A candidate who has secured a minimum of 50% marks in all courses prescribed in the programme and earned a minimum of 72 credits will be considered to have passed the Master's programme.

Grading

A ten point rating scale is used for the evaluation of the performance of the student to provide letter grade for each course and overall grade for the Master's Programme.

Marks	Grade Points	Letter Grade	Class
90	10	S	Exemplary
85-89	9.0	D++	Distinction
80-84	8.5	D+	Distinction
75-79	8.0	D	Distinction
70-74	7.5	A++	First Class
65-69	7.0	A+	First Class
60-64	6.5	A	First Class
55-59	6.0	B	Second Class
50-54	5.5	C	Second Class
49 or Less		F	Fail

The successful candidates are classified as follows.

I – Class 60% marks and above in overall percentage of marks (OPM).

II – Class 50-59% marks in overall percentage of marks.

Candidates who obtain 75% and above but below 90% of marks (OPM) shall be deemed to have passed the examination in FIRST CLASS (Distinction) provided he/she passes all the course prescribed for the programme at the first appearance.

Course-Wise Letter Grades

The percentage of marks obtained by a candidate in a course will be indicated in a letter grade.

A student is considered to have completed a course successfully and earned the credits if he/she secures an overall letter grade other than F. A letter grade F in any course implies a failure in that course. A course successfully completed cannot be repeated for the purpose of improving the Grade Point.

The F Grade once awarded stays in the grade card of the student and is not deleted even when he/she completes the course successfully later. The grade acquired later by the student will be indicated in the grade sheet of the Odd/Even semester in which the candidate has appeared for clearance of the arrears.

If a student secures F grade in the Project Work / Field Work / Practical Work / Dissertation, he/she shall improve it and resubmit it if it involves only rewriting incorporating the clarification of the evaluators or he/she can re-register and carry out the same in the subsequent semesters for evaluation.

M. Sc CHEMISTRY

I year Course code	Course Title	Credit L T/S P C	Inter. Mark	Exter. Mark	Total
First Semester					
CHEC 101	Organic Chemistry I	4 0 0 4	25	75	100
CHEC 102	Inorganic Chemistry I	4 0 0 4	25	75	100
CHEC 103	Physical Chemistry I	4 0 0 4	25	75	100
Second Semester					
CHEC 201	Organic Chemistry II	4 0 0 4	25	75	100
CHEC 202	Inorganic Chemistry II	4 0 0 4	25	75	100
CHEC 203	Physical Chemistry II	4 0 0 4	25	75	100
STAO 215.5	Statistical Methods	4 0 0 4	25	75	100
CHEP 204	Organic Practical I (I & II Semesters)	0 0 4 4	40	60	100
CHEP 205	Inorganic Practical I (I & II Semesters)	0 0 4 4	40	60	100
CHEP 206	Physical Practical I (I & II Semesters)	0 0 4 4	40	60	100
Third Semester					
II year Course code	Course Title	Credit L T/S P C	Inter. Mark	Exter. Mark	Total
CHEC 301	Synthetic Organic Chemistry	4 0 0 4	25	75	100
CHEC 302	Analytical Techniques	5 0 0 5	25	75	100
CHEC 303	Spectroscopy and Spectrometry	5 0 0 5	25	75	100
BIOO 315	Biochemistry	4 0 0 4	25	75	100
ENGE 316	Soft Skill Development	4 0 0 4	25	75	100
Fourth Semester					
CHEC 401	Advanced Organic Chemistry	4 0 0 4	25	75	100
CHEC 402	Advanced Physical Chemistry	4 0 0 4	25	75	100
CHEC 403.1	Chemistry of Advanced Materials (OR)	4 0 0 4	25	75	100
CHEC 403.2	Advanced Inorganic Chemistry	4 0 0 4	25	75	100
CHEC 404.1	Applied Chemistry (OR)	4 0 0 4	25	75	100
CHEC 404.2	Industrial and Medicinal Chemistry	4 0 0 4	25	75	100
CHEP 405	Organic Practical II (III & IV Semesters)	0 0 4 4	40	60	100
CHEP 406	Inorganic Practical II (III & IV Semesters)	0 0 4 4	40	60	100
CHEP 407	Physical Practical II (III & IV Semesters)	0 0 4 4	40	60	100

FIRST SEMESTER
CHEC 101: ORGANIC CHEMISTRY - I

Unit - I Nomenclature, Aromaticity and Electronic Effects

IUPAC nomenclature of annulenes, condensed carbocyclic and aromatic ring systems, heterocyclic rings, polycyclic compounds, spiro compounds and crown compounds.

Non-benzenoid aromatic compounds - Huckel rule - aromaticity of annulenes, heteroannulenes and fullerenes.

Inductive and field effects- mesomeric and hyperconjugative effects – steric inhibition of resonance- influence on strengths of organic acids and bases. Hydrogen bonding and its effects.

Unit - II Organic Reaction Mechanisms - I

Types of organic reactions – Reaction intermediates – formation, structure and stability of carbocations, carbanions, radicals, carbenes and nitrenes.

Aromatic electrophilic substitution – mechanisms of nitration, halogenation and sulphonation reactions. Friedel-Crafts reaction and its modifications. Influence of Cl, Me, OH, NH₂, NHCOCH₃ and NO₂ on reactivity and orientation.

Electrophilic substitution of naphthalene – formation of two isomers – explanation of kinetic and thermodynamic controls by sulphonation of naphthalene.

Aliphatic nucleophilic substitution – S_N1, S_N2 and S_Ni mechanisms – simple examples.(Elementary idea only)

Esterification, hydrolysis and transesterification by acid-catalysed acyl oxygen fission mechanism – explanation of the principle of microscopic reversibility.

Unit - III Stereochemistry - I

Optical isomerism – chirality – asymmetry and dissymmetry - enantiotopic and diastereotopic hydrogens. Enantiomers and diastereomers and their representation by flywedge and Fischer projections – R,S notation

Conformational analysis of 1,2-disubstituted-ethanes – relative stabilities of gauche and anti conformations. Representations of the conformations of diastereomers with two asymmetric carbons using Newmann and Sawhorse projections – relative stabilities of diastereomers.

Geometrical isomerism about C=C bond – E-Z notation – determination of configuration of geometrical isomers – geometrical isomerism in acyclic oximes.

Unit - IV Organic Photochemistry – I

Photochemical reactions of saturated ketones – Norrish type-I & II reactions- photoreductions of ketones- Paterno-Buchi reaction- reaction of α,β unsaturated ketones- isomerisation and cycloadditions - photo reactions of cyclohexadienones.

Photochemical cis-trans isomerisation of simple alkenes – photochemical oxidation, oxidative couplings. Barton reaction.

Unit - V Natural Products - I

Alkaloids - Structure and important biological properties of quinine, papaverine, cocaine, atropine, nicotine and adrenaline – general methods of structural elucidation of alkaloids – structural elucidation and synthesis of papaverine and atropine.

Terpenoids – classification – isoprene rule and special isoprene rule – general methods of structural elucidation of terpenoids – structural elucidation and synthesis of camphor, zingiberene and vetivones.

Text Books and References

1. W. Billmeyer, A Text Book of Polymer Science, Wiley Interscience, 1984.

2. E.L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill, 1962.
3. L.N. Ferguson, The Modern Structural Theory of Organic Chemistry, Prentice Hall, 1963.
4. I. L. Finar, Organic Chemistry, Vol. 1 & 2, ELBS, 1964.
5. P. J. Garrat, Aromaticity, McGraw Hill, 1971
6. R.D. Guthrie, J. Honeyman, An Introduction to the Chemistry of Carbohydrates, Clarendon Press, Oxford, 1964.
7. Jerry March, Advanced Organic Chemistry, Wiley – VCH, Weinheim, 2000.
8. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International, 1991.
9. S.W. Pelletier, Chemistry of Alkaloids, Elsevier, 2001.

CHEC 102: INORGANIC CHEMISTRY - I

Unit - I Molecular Structure

Molecular orbital theory, construction of molecular orbitals in diatomic molecules and triatomic molecules. Molecular orbitals in polar molecules, percentage of ionic character, Bond length and bond energy. Electronegativity - Alred–Rochow and Mulliken–Jaffe electronegativity scales - Group electronegativity, electro neutrality principle.

Structures of BeH_2 , $(\text{CH}_3)_3\text{B}$, COCl_2 , PF_5 , SF_6 , SF_4 , ClF_3 , $(\text{CH}_3)_3\text{P}$, XeF_6 and IF_7 based on VSEPR theory.

Unit - II Solid State Chemistry

Ionic bonding, Lattice energy, Born equation and its derivation, radius ratio rules, structures of some ionic crystals (sodium chloride, caesium chloride, Rutile, Wurtzite, Fluorite). Bonding and structures of electron deficient molecules like boranes and metal alkyls. Electrostatic forces – ion-dipole and dipole-dipole interactions, van der Waals forces.

Unit - III Coordination Chemistry - I

Coordination Chemistry of transition metal ions – Nomenclature – stability constants of complexes and their determination (pH metric and spectrophotometric methods). Factors influencing stability, stabilization of unusual oxidation states by complex formation.

Pearson's HSAB concept, Acid-base strength and hardness and softness. Symbiosis, theoretical basis of hardness and softness. Electronegativity and hardness or softness.

Stereoisomerism of co-ordination complexes.

Unit - IV Coordination Chemistry - II

Bonding in complexes: Metal–ligand bond. Crystal field theory – splitting of d – orbitals, CFSE. Evidence for CFSE. Factors affecting splitting, spectrochemical series, Limitations of CFT, ligand Field Theory, M.O. Theory

Distortions in octahedral complexes. Jahn-Teller distortion – spectral implications of Jahn-Teller distortions in transition metal complexes.

Unit - V Nuclear Chemistry

Radioactive decay and equilibrium. Nuclear Q – value – cross sections, types of reactions; fission and fusion; fission products and fission yields, Modes of radioactive decay: α - and β -decay, orbital electron capture, nuclear isomerism, internal conversion. Hot atom chemistry.

Radioactive techniques, tracer technique, neutron activation analysis, counting techniques such as Geiger Muller, ionization and proportional counters. Applications of nuclear science in agriculture and biology. Atomic power projects in India.

Text Book And References

1. H. J. Arnikar, Essential of Nuclear Chemistry, New Age International, 1995.

2. D. Bannerje, Coordination Chemistry, Tata McGraw – Hill, 1993.
3. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, Wiley Eastern, 1988.
4. B. E. Douglas. D. H. Mc Daniel, J. J. Alexander, Concepts and Models of Inorganic Chemistry, Blaisdell Publishing Company, 1965.
5. B.N.Figgis, Introduction to Ligand Field Theory, Wiley Eastern, 1976.
6. G. Friedlander, J.W. Kennedy, N.M. Miller, Nuclear and Radio Chemistry, John Wiley, 1981.
7. S. Glasstone, Source Book of Atomic Energy, Affiliated East West Press, 1967.
8. S.F.A. Kettle, Coordination Compounds, Publisher Thomas Nelson, 1969.
9. L. Pauling, The Nature of Chemical Bond, Cornell University Press, 1961.

CHEC 103: PHYSICAL CHEMISTRY - I

Unit - I Chemical Kinetics and Catalysis

Absolute Reaction Rate Theory in thermodynamic terms – Significance of entropy and volume of activation. Ionic reactions – primary and secondary salt effects - Acid-base catalysis – Bronsted relations, catalytic coefficients and their determination. Enzyme catalysis - Michaelis-Menten equation – Heterogeneous catalysis-Langmuir-Hinshelwood and Eley-Rideal mechanisms

General features of fast reactions – Study of fast reactions by flow methods

Unit - II Photochemistry and Radiation Chemistry

Jablonski diagram, primary and secondary processes, Quantum yield. Photosensitization, Chemiluminescence. Kinetics of collisional quenching – Stern Volmer equations. Photosynthesis, solar energy conversions. Semiconductor photocatalysis, flash photolysis, lasers.

Radiation Chemistry-linear energy transfer, G-value, dosimeters, radiolysis of water, solvated electrons.

Unit - III Group Theory

Symmetry operations, point groups, reducible and irreducible representations, orthogonality theorem. Construction of C_{2v} and C_{3v} character tables. Selection rules for IR and Raman spectra, procedure for determining symmetry of normal modes of vibration - hybrid orbitals in BF_3 , CH_4 , NH_3 and SF_6 .

Unit - IV Spectroscopy

Origin of Molecular spectra - rotational spectra - rigid rotor and non-rigid rotor – Effect of isotopic substitution. Vibrational spectra – harmonic and anharmonic oscillators – fundamental vibrations and overtones – hot bands. Vibrational-rotational spectra – P, Q, R branches. Electronic spectra of diatomic molecule – Potential energy curves – Franck-Condon Principle.

Raman spectra – theory – Selection Rules – Rotational Raman Spectra and Vibrational Raman Spectra. Mutual exclusion principle.

Unit - V Electrochemistry - I

Debye-Huckel-Onsager equation and its verification, conductance at high field and high frequency. Debye-Huckel limiting law.

Electrochemical cell reactions, Nernst equation – electrochemical series. Electrode-electrolyte interface – Electrokinetic Phenomena. Batteries, Fuel cells, corrosion and its prevention.

Text Books and References

1. G.L.Agarwal, Basic Chemical Kinetics, Tata McGraw Hill, 1990.
2. C.N.Banwell, Fundamentals of Molecular Spectroscopy, Tata McGraw Hill, 1993.
3. F. A. Cotton, Chemical Applications of Group Theory, Wiley Eastern, 1971.
4. S. Glasstone, An Introduction to Electrochemistry, Affiliated East West Press, 1971.

5. S. Glasstone, Text Book of Physical Chemistry, Mc Millan, 1956.
6. K. J. Laidler, Chemical Kinetics, Tata Mc Graw Hill, 1990.
7. W. J. Moore, Basic Physical Chemistry, Prentice Hall, 1986.
8. K. V. Raman, Group Theory and its Application to Chemistry, Tata McGraw Hill, 1994.
9. K.K. Rohatgi Mukherjee, Fundamentals of Photochemistry, Wiley Eastern, 1987.

SECOND SEMESTER
CHEC 201: ORGANIC CHEMISTRY - II

Unit - I Stereochemistry- II

Walden inversion, asymmetric induction and asymmetric transformation - enantio and diastereo selective synthesis – enantiomeric excess and diastereomeric excess.

Atropisomerism of biphenyls, allenes and spiranes

Conformational analysis of cyclohexane and its mono-and di-substituted derivatives.

Unit - II Photochemistry – II

Classification of pericyclic reactions, electrocyclic reactions of 1,3-dienes, di- π methane rearrangement, sigmatropic rearrangement

Selection rules and stereochemistry of electrocyclic reactions, cycloadditions and sigmatropic shift, Sommet-Hauser, Cope and Claisen rearrangements

Unit - III Organic Reaction Mechanisms - II

Aliphatic electrophilic substitution - S_E1 , S_E2 and S_{Ei} mechanisms, electrophilic substitution with migration of double bond.

Aromatic nucleophilic substitution: Unimolecular, bimolecular and benzyne mechanisms.

Addition to carbon-carbon and carbon-oxygen multiple bonds – electrophilic and nucleophilic addition – addition to conjugated system. Hydration of olefins – Hydroboration

Elimination reactions: $E1$, $E2$, $E1cB$ & $E2C$ mechanisms – Pyrolytic eliminations – cis elimination - orientation of double bond – Bredt's rule, Hofmann & Saytzeff rules.

Unit - IV Natural Products - II

Structural elucidation of sucrose and maltose, structures of starch and cellulose - Amino acids – classification, general methods of preparation and general properties of amino acids.

Proteins – classification, primary structure of peptides, end group analysis.

Classification of enzymes and their specificity.

Ribonucleosides and ribonucleotides –RNA - types -structures of DNA and RNA.

Unit - V Synthetic Dyes and Polymers

Colour and constitution (Electronic concept). Classification of dyes, Chemistry and Synthesis of methyl orange, congo red, malachite green, crystal violet, phenolphthalein, fluorescein, alizarin and indigo

Polymers – Chemistry of polymerisation, Molecular weight and size, Kinetics of polymerisation, Chemical and geometrical structure of polymer molecules, Glass transition temperature, Crystallinity in polymers and Copolymerisation.

Text Book and References

1. S.P.Singh, S.M.Mukherjee, Organic Reaction Mechanisms, Macmillan, 1984.
2. P. Sykes, Guide Book to Mechanism in Organic Chemistry, Prentice Hall, 6th Edition, 1986.
3. R .K. Bansal, Organic Reaction Mechanisms, New Age international, 1996.
4. F. A. Carey, R. J. Sunberg, Advanced Organic Chemistry, Part A, Springer, 5th Edition, 2007.
5. I. L. Finar, Organic Chemistry, Vol.II , ELBS, 1977.

6. E. L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill, 1962.
7. J.M.Coxton & B.Halton, Organic Photochemistry, Cambridge University Press, 2nd Edition, 2011.
8. E.C.H. Depuy, O.S. Chapman, Molecular Reactions and Photochemistry, Prentice Hall, 1975.
9. Stuart Warren, Designing Organic Synthesis, Wiley-VCH, 1982.
10. R. O. C. Norman, Modern Methods in Organic Synthesis, Macmillan, 1967
11. V.R.Gowariker, N.V.Viswanathan, N.V.Jayadev Sreedhar, Polymer Science, New Age International (P) Limited, Publishers, 2005.

CHEC 202: INORGANIC CHEMISTRY - II

Unit - I Lanthanides and Actinides

Correlation of electronic structures, occurrence and isolation, separation - Chemistry of separation of Np, Pu & Am from U & fission products. Oxidation states and general properties – Comparison with 'd' block elements, Lanthanide contraction and its significance, Coordination compounds of lanthanides - Spectral and magnetic characteristics of lanthanides and actinides - Position in the periodic table. Similarities between the actinides and lanthanides

Unit - II Organometallic Chemistry - I

Synthesis and structure of metal complexes with alkenes and alkynes, bonding in such complexes, use of organometallic reagents in hydrogenation, hydroformylation, isomerisation and polymerization reactions.

Activation of small molecules by co-ordination.

Unit - III Bioinorganic Chemistry

Role of alkali and alkaline earth metals in biological systems and their transport across the membranes – Ionophores – Metalloporphyrins – cytochromes – ferredoxins. Physiology of myoglobin and haemoglobin – Dioxygen binding. Electron transfer, respiration and photosynthesis - PS-I, PS-II – Vitamin B₁₂ and B₁₂ coenzymes - Nitrogen fixation.

Unit - IV Organometallic Chemistry - II

Metal carbonyls – 18-Electron rule – M.O. theory, Polynuclear carbonyls with and without bridging groups – carbonylate anions – carbonyl hydrides – metal nitrosyls – dinitrogen complexes. Metallocenes: preparation, properties, structure and bonding of ferrocene like compounds. Complexes of cyclohexadienyl molecules.

Unit - V Photoinorganic Chemistry

Excited states of metal complexes – Energy transfer under conditions of weak interaction and strong interaction – exciplex formation. Conditions of the excited states to be useful as redox reactants - photosubstitution, photooxidation and photoreduction – photochemical reactions involving Ruthenium(II) –bipyridyl complex. Comparison with [Fe(bipy)₃]⁺² – Application to photovoltaics – Water photolysis – carbon dioxide reduction.

Text Books and References

1. G. L. Ferraudi, Elements of Inorganic Photochemistry, Wiley Eastern, 1988.
2. E. A. V. Ebsworth, D.W.H. Rankine, S.Craddock, Structural Methods in Inorganic Chemistry, ELBS, 1991.
3. J. E. Huheey, Inorganic Chemistry, Addison Wesley, 1993.
4. B.E.Douglas, D.H.McDaniel, J.J.Alexander, Concepts and Models of Inorganic Chemistry, John Wiley and Sons, Blaisdell Publishing co., 1965.
5. F. A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, Wiley Eastern, 1988.
6. L. Pauling, The Nature of Chemical Bond, Cornell University Press, 1961.

7. S.F.A. Kettle, Coordination Compounds, ELBS, 1975.
8. S.F.A. Kettle, Physical Inorganic Chemistry – A Coordination Chemistry Approach, Springer, 1992.
9. D.L.Nelson, M.M.Cox, Lehninger Principles of Biochemistry, W. H. Freeman and Co., 5th Edition, 2008.
10. G. N. Mukherjee, Elements of Bio-inorganic Chemistry, 4th Edition, U.N. Dhur and Sons, 1993.
11. G. L. Eichhorn, Inorganic Biochemistry, Elsevier Science Publication, 1973.
12. Vincenzo Balzani, Alberto Juris, Photochemistry and Photophysics of Ru(II) polypyridine complexes in the Bologna group. From early studies to recent developments, Coordination Chemistry Reviews, 211 (2001) 97-115.

CHEC 203: PHYSICAL CHEMISTRY - II

Unit - I Thermodynamics - I

Calculation of adiabatic flame temperature, Maxwell's relations, thermodynamic equation of state, thermodynamics of open systems, partial molar quantities, chemical potential, Gibbs-Duhem equation, variation of chemical potential with temperature and pressure, third law of thermodynamics, Nernst heat theorem, chemical equilibrium-Van't Hoff reaction isotherm, standard free energy change of reactions, variation of equilibrium constant with temperature and pressure.

Unit - II Thermodynamics - II

Fugacity of gases – determination of fugacity using graphical method and Van der Waals' equation – variation of fugacity with temperature and pressure. Concept of activity and activity coefficients – mean ionic activity and mean activity coefficients - determination of activity and activity coefficients using EMF measurements.

Non-equilibrium thermodynamics - conservation of energy and mass, entropy production – Microscopic reversibility and Onsager reciprocal relation. General application of non-equilibrium thermodynamics.

Unit - III Quantum Chemistry - I

Planck's quantum theory, wave particle duality, uncertainty principle, operators and commutation relations-Postulates of quantum mechanics – derivation of Schrodinger's time-independent wave equation and its application to particle in a one-dimensional box, particle in a three-dimensional box, harmonic oscillator, rigid rotor and hydrogen atom.

Unit - IV Quantum Chemistry - II

Covalent bonding – Born-Oppenheimer approximation-Hydrogen molecule ion, LCAO – MO and VB treatments of the hydrogen molecule. Antisymmetry and Pauli's exclusion principle. Slater determinantal wave function, term symbols and spectroscopic states – Russell-Saunders coupling.

Unit - V Material Science

Band theory - insulators, semiconductors and conductors and their applications - superconductors and their applications – A study of conducting polymers, liquid crystals, non-linear optical materials and photochromic materials and their applications.

Text Books and References

1. A.K. Chandra, Introduction to Quantum Chemistry, Tata McGraw Hill, 1997.
2. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, New Delhi, 1960.
3. W. Levine, Quantum Chemistry, Prentice Hall, 1994.
4. S.H. Maron, C.F. Prutton, Principles of Physical Chemistry, McMillan, 1960.

5. W.J. Moore, Basic Physical Chemistry, Prentice Hall, 1986.
6. R. K. Prasad, Quantum Chemistry, Wiley Eastern, 1993.
7. J.C.Kuriacose, J. Rajaram, Thermodynamics for Chemistry, Shoban Lal Nagain Chand, New Delhi, 1986.
8. B.K. Sen, Quantum Chemistry, Tata McGraw Hill, 1992.

STAO 215.5: STATISTICAL METHODS

Unit – I

Definition, scope, functions and limitations of Statistics – Collection, Classification, Tabulation of data, Diagrammatic representation of data – Simple, Multiple and Percentage Bar diagram, Pie diagram and Graphical representation of data – Histogram, frequency polygon, frequency curve and ogives. Primary and Secondary data – Questionnaire method.

Unit – II

Measures of Central tendency – Mean, Median and Mode and their practical usages. Measures of Dispersion: Range, Quartile Deviation, Mean Deviation, Standard Deviation, Variance and Coefficient of Variation. Measures of Skewness – Pearson's, Bowley's method. Applications of Binomial and Normal distributions.

Unit – III

Measure of Bivariate data – Simple, Partial and Multiple Correlation. Scatter diagram and Pearson's method, Rank correlation. Regression and their equations – Prediction. Basic concept of Sampling – Parameter and Statistics – Sampling distribution and Standard Error – Simple random sampling and stratified random sampling.

Unit – IV

Tests of Significance with their important concepts. Tests for large samples - Test for mean, difference of means, proportion and equality of proportions. Small sample tests – Test for mean, difference of Means, paired samples, test for correlation and regression coefficients, Chi square test for goodness of fit and independence of attributes.

Unit - V

Applications and analysis using SPSS – Analysis of variance one way and two way classifications. Multiple regression analysis, Logistic regression analysis, Factor analysis, Cluster analysis, Discriminant function analysis.

Note: The emphasis is only on the application of the methods. The derivations of the formulae are not necessary.

Text Books and References

1. S.P. Gupta, Statistical Methods, Sultan Chand & Sons, Pvt. Ltd, New Delhi, 2011.
2. S.C. Gupta, V.K. Kapoor, Fundamentals of Mathematical Statistics, Sultan Chand & Sons, Pvt. Ltd, New Delhi, 2011.
3. Darren George, Paul Mallery, SPSS for Windows, 10th Edition, Pearson, 2011.

CHEP 204: ORGANIC CHEMISTRY PRACTICAL - I

Preparations : Preparations involving reactions such as nitration, diazotisation, oxidation and reduction.

Qualitative Analysis : Analysis of two component mixtures. Separation and systematic analysis of two component mixtures.

CHEP 205: INORGANIC CHEMISTRY PRACTICAL – I

Complexometric Titrations

- Standardization of EDTA.
- Determination of Mg^{2+} , Zn^{2+} , Ni^{2+} and Ca^{2+}
- Hardness of water.

Semi Micro Qualitative Analysis

Mixture containing two common cations and two of the following less familiar cations.
Se, Te, W, Mo, Be, Ti, Ce, Th, Zr, U, V, Tl and Li.

CHEP 206: PHYSICAL CHEMISTRY PRACTICAL - I

I. Conductivity

- Determination of cell constant
- Determination of the solubility of sparingly soluble salt
- Verification of DHO equation – Equivalent conductance of strong electrolyte
- Dissociation constant of weak electrolyte (Verification of Ostwald's dilution law)

II. Conductometric titrations

- Acid-base titrations
 - HCl vs NaOH, ii) CH_3COOH vs NaOH, iii) $HCl + CH_3COOH$ vs NaOH
- Displacement titrations (NH_4Cl vs NaOH)
- Precipitation titrations
 - $CuSO_4$ vs NaOH, ii) $BaCl_2$ vs Na_2CO_3 , iii) KCl vs $AgNO_3$

III. Phase Rule : Two component system: Simple Eutectic

IV. Distribution Law

- Partition coefficient of iodine between two immiscible solvents
- Study of the equilibrium constant of the reaction : $KI + I_2 \rightleftharpoons KI_3$
- Distribution of ammonia between water and chloroform
- Determination of formula of cuprammonium complex

THIRD SEMESTER

CHEC 301: SYNTHETIC ORGANIC CHEMISTRY

Unit - 1 Reagents In Organic Chemistry

Uses of the following reagents in organic synthesis and functional group transformations.

Sodium borohydride, Lithium aluminium hydride, tri-n-butyl tin hydride, Lithium dimethyl cuprate, Lithium diisopropyl amide, Trimethyl silyl iodide, dicyclohexylcarbodiimide, OsO_4 , DDQ, SeO_2 , PCC.

Phase Transfer Catalysts – Benzyltriethylammonium halides – Crown ethers.

Unit - II Organic Reactions - I

Formation of C-C single bond: Aldol condensation, Claisen ester reaction, Stobbe condensation, Knoevenagel reaction, Michael addition, Dieckmann condensation – Stork enamine reaction – Mannich reaction, Reformatsky reaction

Formation of C=C double bond: Wittig reaction, Perkin reaction, Claisen – Schmidt condensation, Peterson's synthesis.

Unit - III Organic Reactions - II

Cannizzaro and cross Cannizzaro reactions, Benzoin condensation, Wolff-Kishner reduction, Clemmenson reduction, MPV reduction, Birch reduction. Riemer-Tiemann reaction – Gattermaan reaction - Chichibabin reaction. Uses of organoboron compounds in organic synthesis. Some industrial applications of organic reactions.

Unit - IV Selective Synthetic Methods

Need for protection of functional groups during chemical reactions – protection of hydroxyl, mercapto, amino, carbonyl and carboxylic groups.

Regioselective synthesis – halogenation of alkanes, ambident nucleophiles, Regiospecific synthesis – reductions using Baker's yeast.

Stereo selective reaction – bromination of dicarboxyacetylene, Sharpless asymmetric epoxidation, synthesis of 2-butanol by using diisopinocampylborane.

Stereospecific reaction – bromination of fumaric and maleic acids.

Unit - V Planning Organic Synthesis

An introduction to retrosynthesis - Synthons, Synthetic equivalent, Target molecule, Functional group interconversion - Disconnection approach – One group disconnection – Disconnection of alcohols, olefins and ketones - Logical and illogical disconnections. Two group disconnection-1,2-, 1,3-, 1,4-, 1,5- and 1,6-dioxygenated skeletons and dicarbonyls. Retro Diels – Alder reaction – Pericyclic reactions – Retrosynthesis of some heterocycles containing two nitrogen atoms.

Retrosynthetic analysis of Camphor, Longifiline, Reserpine and Cortisone

Text Book and References

1. R.K. Bansal Organic Reaction Mechanisms, New Age International, 1996.
2. F.A. Carey, R. J. Sunberg, Advanced Organic Chemistry Part A, Springer, 5th edition, 2007
3. W. Carruthers, Some Modern Methods in Organic Synthesis, Cambridge, 1971
4. E.J. Corey, Reactions and Reagents in Organic Synthesis, VCH, 1988
5. C.H. Depuy, O.S. Chapman, Elements of Organic Photochemistry, Prentice Hall, 1975.
6. I.L. Finar, Organic Chemistry Vol.II, ELBS, 1977.
7. R.O.C. Norman, Modern Methods in Organic Synthesis, Macmillan, 1967
8. S.P. Singh, S.M. Mukherjee, Reaction Mechanisms in Organic Chemistry, Macmillan, 1984
9. P. Sykes, Guide Book to Mechanism in Organic Chemistry, Prentice Hall, 6th Edition, 1986.

CHEC 302: ANALYTICAL TECHNIQUES

Unit - I Electroanalytical Methods

Principles and application of electrogravimetry, coulometry – amperometry – potentiometry – conductometry – polarography – voltammetry – cyclic voltammetry – anodic stripping voltammetry.

Unit - II Photoelectron And ESR Spectroscopies

Valence and core binding energies – Measurement technique – Koopman's theorem – Chemical shifts in X-ray photoelectron spectroscopy – Auger spectroscopy – Applications of ESCA in chemistry.

Electron spin Resonance Spectroscopy – Origin of the spectrum – method of recording - hyperfine splitting – g value and hyperfine splitting constant - ESR spectra of simple organic radicals - application of ESR spectra to transition metal complexes

Unit - III NQR and Mossbauer Spectroscopies

NQR spectroscopy – Theory of NQR – instrumentation – Nuclear quadrupole coupling constants – Applications.

Mossbauer spectroscopy – principle – source and absorber – isomer shift – quadrupole splitting – magnetic interactions – applications to Fe and Sn compounds.

Unit - IV Diffraction Methods

X-ray diffraction – structures of simple lattices and X-ray intensity – structure factor and its relation to electron density – Identification of unit cells from systematic absence – practical application of single crystal photography – Powder pattern.

Electron and neutron diffractions – scattering intensity vs scattering angle – Wierl equation - scattering of neutrons by solids and liquids – Magnetic scattering – measurement techniques – comparison with X-ray diffraction – Elucidation of structures of simple gas phase molecules.

Unit - V Chromatography and ORD

Principles of gas – liquid and gas – solid chromatography – Instrumentation - Applications – Principles and Applications of HPLC – super critical fluids chromatography – Properties of super critical fluids – Instrumentation and applications.

Theories of optical rotatory dispersion and circular dichroism – correlation between structure and optical rotation – axial haloketone rule – Cotton effect – Octant rule – Deduction of absolute configuration of organic molecules and inorganic complexes.

Text-Books and References

1. R.A.Day, A. L. Underwood, Quantitative Analysis, Prentice Hall,1999.
2. R.S. Drago, Physical Methods in Chemistry, Saunders, 1999.
3. E. A. V. Ebsworth, D.W.H. Rankine, S.Craddock, Structural Methods in Inorganic Chemistry, ELBS, 1991.
4. J.H.D.Eland, Butterworth, Photoelectron Spectroscopy, 2nd Edition, Elsevier, 1983.
5. E.L. Eliel, Stereochemistry of Carbon Compounds, Tata McGraw Hill, 1962.
6. D.G.Peters, J. M.Hayes, G. M. Hefige, A Brief Introduction to Modern Chemical Analysis, Saunders, 1976.
7. Douglas A. Skoog, F. James Holler, Timothy A. Nieman, Principles of Instrumental Analysis, Saunders Cllee Pub., 1998.
8. H.H. Willard, L.L. Merrit, J.A. Dean, Instrumental Methods of Analysis, W.B. Saunder, 1987.

CHEC 303: SPECTROSCOPY AND SPECTROMETRY

Unit - I UV and IR Spectroscopy

Ultraviolet – Visible spectroscopy – types of electronic transitions – chromophores and auxochromes - factors influencing positions and intensity of absorption bands – absorption spectra of dienes, polyenes and α , β - unsaturated carbonyl compounds – Woodward – Fieser rules.

IR Spectroscopy – vibrational frequencies and factors affecting them – identification of functional groups – intra and inter molecular hydrogen bonding – finger print region – Far IR region – metal ligand stretching vibrations.

Unit - II NMR Spectroscopy

Nuclear spin – magnetic moment of a nucleus – nuclear energy levels in the presence of magnetic field, relative populations of energy levels – macroscopic magnetization – basic

principles of NMR experiments – CW and FT NMR – ^1H NMR – chemical shift and coupling constants – factors influencing proton chemical shifts and vicinal proton – proton coupling constants – ^1H NMR spectra of simple organic molecules such as: $\text{CH}_3\text{CH}_2\text{Cl}$, CH_3CHO , etc., AX and AB spin system – spin decoupling – nuclear Overhauser effect – chemical exchange.

Unit - III ^{13}C NMR and Two - Dimensional NMR Spectroscopies

^{13}C NMR – proton decoupled and off-resonance ^{13}C NMR spectra – factors affecting ^{13}C chemical shifts – ^{13}C NMR spectra of simple organic molecules – Basic principles of two-dimensional NMR spectroscopy – HOMOCOSY, NOESY and HSQC spectra and their applications (No pulse sequence is expected).

Unit - IV Mass Spectrometry

Principles – measurement techniques – (EI, CI, FD, FAB, SIMS) – presentation of spectral data – molecular ions – isotope ions – fragment ions of odd and even electron types – rearrangement ions – factors affecting cleavage patterns – simple and multicentre fragmentation – McLafferty rearrangement – Retro Diels–Alder fragmentation. Mass spectra of hydrocarbons, alcohols, phenols, aldehydes, ketones, carboxylic acids, amines and their derivatives.

Unit - V Spectroscopic identification of Organic Compounds

Identification of organic compounds using UV, IR and NMR spectroscopy and mass spectrometry - problems.

Text Books and References

1. D. Dyer, Application of Absorption Spectroscopy of Organic Compounds, Prentice Hall, 1978.
2. V. Fibrolein, Basic and Two Dimensional NMR Spectroscopy, 1982.
3. William Kemp, Organic Spectroscopy, 3rd edition, Macmillan, 1989.
4. J.B. Lambert, H. F.Shurrell, A. P. Lightner, R. G. Cooks, Introduction to Organic Spectroscopy, Macmillan, 1987.
5. Robert M. Silverstein, F.X. Webster, Spectrometric Identification of Organic Compounds, John Wiley, 1998.
6. J.B. Stothers, Carbon -13 NMR Spectroscopy, Academic Press, 1972.

BIOO 315: BASIC BIOCHEMISTRY

Unit – I

Classification of carbohydrates. Functions of biologically important mono saccharides, disaccharides, homo polysaccharides, and hetero polysaccharides. Carbohydrate metabolism: glycolysis, citric acid cycle, gluconeogenesis, glycogen metabolism (overview only, structures not required). Diabetes mellitus (elementary details).

Unit – II

Amino acids: classification and acid-base properties. Biologically important peptides. Proteins– classification, functions, denaturation and renaturation. Orders of protein structure: Primary, secondary (α -helix, β -pleated sheet), supersecondary, tertiary, and quaternary structures. Urea cycle, (overview only, structures not required).

Unit – III

Classification of lipids. Structure and functions of cholesterol. Lipid metabolism: β -oxidation of fatty acids, biosynthesis of fatty acids (overview only, structures not required). Coronary heart disease (elementary details).

Unit – IV

Enzymes: Classification and nomenclature. Specificity, factors affecting enzyme activity- substrate, pH and temperature. Michaelis - Menten equation and L-B plot. Coenzymes and Isoenzymes (brief account only). Allosteric enzymes. Applications of enzymes in clinical diagnosis, therapeutics and industry.

Unit – V

DNA structure- Watson and Crick model. A, B, and Z forms of DNA. DNA denaturation. Differences between DNA and RNA. Major classes of RNA- structure and biological functions.

Text Books

1. D.L.Nelson, M.M.Cox, Lehninger Principles of Biochemistry, Freeman, 6th edition, 2012.
2. R.K. Murray et al., Harper's Illustrated Biochemistry, 30th edition, McGraw Hill, 2015.
3. U. Satyanarayana, Biochemistry, Allied Publishers, latest edition.

ENGE 316: SOFT SKILL DEVELOPMENT

Unit - 1: Soft Skills and Personality Development

Soft Skills: Meaning and Importance - Hard Skills versus Soft Skills - Self Concept: Self Awareness, Self Development and Self Realisation – Power of Positive Attitude – Etiquette and Manners.

Listening: Types of Listening, Effective Listening and Barriers to Listening – Assertive Communication.

Unit - 2: Communication Skills

Oral Communication: Forms, Types of Speeches and Public Speaking – Presentation: Elements of Effective Presentation and Use of Visual Aids in Presentation.

Written Communication: Strategies of Writing – Business Letters: Form, Structure and Formats – Types of Business Letters – Memos – Agenda and Minutes.

Non-verbal Communication: Body Language and Proxemics.

Unit - 3: Interpersonal Skills

Interpersonal Skills: Relationship Development and Maintenance and Transactional Analysis. Conflict Resolution Skills: Levels of Conflict and Handling Conflict - Persuasion – Empathy – Managing Emotions – Negotiation: Types, Stages and Skills – Counselling Skills.

Unit - 4: Employability Skills

Goal Setting – Career Planning – Corporate Skills – Group Discussion – Interview Skills – Types of Interview - Email Writing – Job Application – Cover Letter - Resume Preparation.

Unit - 5: Professional Skills

Decision Making Skills – Problem Solving – Emotional Intelligence – Team Building Skills – Team Spirit – Time Management – Stress Management: Resolving Techniques.

References:

1. B.N. Ghosh, *Managing Soft Skills for Personality Development* (Ed). New Delhi, Tata McGraw Hill Education Pvt. Ltd., 2012.
2. Krishna Mohan, Meera Banerji, *Developing Communication Skills*, 2nd Edition, New Delhi MacMillan Publishers India Ltd., 2009.
3. Neera Jain, Shoma Mukherji, *Effective Business Communication*, New Delhi, Tata McGraw Hill Education Pvt. Ltd., 2012.
4. M.S. Rao, *Soft Skills - Enhancing Employability: Connecting Campus with Corporate*, New Delhi, I.K International Publishing House Pvt. Ltd., 2011.

5. M. Ashraf Rizwi, *Effective Technical Communication*, New Delhi, Tata McGraw Hill Education Pvt. Ltd., 2010.
6. Bretag Tracey, Crossman Joanna, Bordia Sarbari, *Communication Skills*, New Delhi, Tata McGraw Hill Education Pvt. Ltd., 2012.

FOURTH SEMESTER

CHEC 401: ADVANCED ORGANIC CHEMISTRY

Unit - I Steroids and Hetrocycles

Occurrence- Diel's hydrocarbon - nomenclature and stereochemistry of Steroids.

Sterols: Structural elucidation of cholesterol and cholic acid.

Sex hormones: Estrogens: Structural elucidation and synthesis of estrone, estradiol and estriol. Gestogens: progesterone – synthesis from cholesterol. Androgens: testosterone and androstrone – Structural elucidation based on their synthesis from cholesterol.

Preparation and reactions of indole, quinoline and isoquinoline with special reference to Fisher indole synthesis, Skraup synthesis and Bischler-Napieralski synthesis.

Unit - II Modern Synthetic Methods

Catalysed synthetic processes including heterogeneous catalysts, a brief description of phase transfer catalysis, misceller catalysis, organic reactions in organized media, polymer supported reagents and Merrifield synthesis. Electro organic synthesis, microwave assisted organic synthesis and an introduction to sonochemistry .

Unit - III Molecular Rearrangements

Nature of migration, migratory aptitude, memory effects. A detailed study of the following rearrangements: Carbon- carbon migration - Pinacol- Pinacolone, Wagner- Meerwein and Favorskii, Carbon-nitrogen migration - Hoffmann, Schmidt, Lossen, Curtius and Beckmann, Carbon- oxygen migration - Baeyer-Villiger.

Unit - IV Organic Reaction Mechanisms - III

General methods of investigation of organic reaction mechanisms – kinetic and non-kinetic methods- Baldwin rules – cross over experiments – isotopic labeling primary and secondary kinetic isotopic effects – solvent kinetic isotopic effects. S_N1' , S_N2' , S_Ni mechanisms - Neighbouring group participation - non-classical carbocation - structure and solvent effect on nucleophilic substitution reactions

Unit - V Advanced Stereochemistry, Antibiotics and Vitamins

Conformation and reactivity in cyclohexane derivatives – conformation analysis of decalines. Secondary structure of peptides.

Antibiotics: classification, structure and uses of penicillins, cephalosporins, chloramphenicol, streptomycin and tetracyclins - Structural elucidation and synthesis of penicillin G and chloroamphenicol.

Vitamins: classification, structure and uses of vitamins A, B₁, B₂, B₆, C, D, E and K Structural elucidation and synthesis of vitamins A, B₁, B₆ and C.

Text Book and References

1. A.Berger, Medicinal Chemistry, Vol.1 & 2, 1st edition, Wiley Interscience, 2003
2. F.A. Carey, R.J. Sundberg, Advanced Organic Chemistry, Section A, 5th edition, Springer, 2007
3. I.L. Finar, Organic Chemistry, Vol. II, ELBS, 1977.
4. W. Carruthers, Some Modern Methods of Organic Synthesis, 4th edition, Cambridge Univ. Press., 2004.

5. H.O. House, Modern Synthetic Reactions, Published by W. A. Benjamin., 1972
6. R.O.C. Norman, Modern Methods in Organic Synthesis, Macmillan, 1967
7. A.R. Pinder, Chemistry of Terpenes, Macmillan, 1962
8. C.W. Shoppee, The Chemistry of Steroids, Published by Butterworth Scientific, New York, 1958.

CHEC 402: ADVANCED PHYSICAL CHEMISTRY

Unit - I Electrochemistry - II

Ion-solvent interactions – Born Model, Enthalpy, free energy and entropy of ion-solvent interactions. Primary and secondary solvations (salting in and salting out). Electrode kinetics – Butler Volmer equation, Tafel equation.

Surface electrochemistry. Electrical double layer, Helmholtz-Perrin, Gouy- Chapman, Stern Theories, Lippmann equation.

Unit - II Quantum Chemistry - III

The variation Theorem, linear variation principle, Perturbation Theory (first order and non degenerate). Applications of variation method and perturbation theory to the helium atom. Hybridization-determination of bond angles of sp , sp^2 and sp^3 hybridizations. Huckel pi-electron theory and its applications to ethylene, butadiene and benzene. A brief idea of self consistent fields.

Unit - III Statistical Thermodynamics

Thermodynamic probability and entropy. Maxwell-Boltzmann, Bose-Einstein and Fermi-Dirac statistics.

Partition function – translational, rotational, vibrational and electronic partition functions. Calculations of thermodynamic properties and equilibrium constant in terms of partition functions. Theories of heat capacity of solids.

Unit - IV Chemical Dynamics

Potential energy surfaces - Dynamics of unimolecular reactions – Lindemann-Hinshelwood – Rice Ramsperger Kassel (RRK) theory and Rice Ramsperger Kassel – Marsus (RRKM) theory

Study of fast reactions by laser - flash Photolysis and the nuclear magnetic resonance method.

LFERs – Hammett equation, Taft equation, separation of polar, resonance and steric effects.

Unit - V Surface Chemistry and Macromolecules

Langmuir and BET Isotherms. Adsorption from solutions – Gibbs adsorption isotherm. Study of surface films – surface area determination – Applications of adsorption – adsorption indicators. Surfactant and detergents. Micelle – critical micellar concentrations–applications.

Macromolecules–number average and weight average molecular weights. Determination of molecular weight. Kinetics of polymerizations.

Text books and References:

1. J.O.M. Bockris, A.K.N. Reddy, Electrochemistry, Volumes 1 & 2, Plenum, New York, 1977.
2. W. Levine, Quantum Chemistry, Prentice Hall, 1994.
3. A. K. Chandra, Introduction to Quantum Chemistry, Tata McGraw Hill, 1997
4. R.K. Prasad, Quantum Chemistry, Wiley Eastern, 1993.
5. B.K. Sen, Quantum Chemistry, Tata McGraw Hill, 1992
6. S. Glasstone, An Introduction to Electrochemistry, Affiliated East West Press, New Delhi, 1977.
7. S. Glasstone, Thermodynamics for Chemists, Affiliated East West Press, New Delhi, 1960.
8. J.Rajaram, J.C. Kuriacose, Thermodynamics for Chemistry, Shoban Lal Nagain Chand, New Delhi, 1986.

9. J.I. Steinfeld, J.S. Francisco, William L. Hass, Chemical Kinetics and Dynamics, Prentice Hall, New Jersey, 1986.
10. K.J. Laidler, Chemical Kinetics, Tata McGraw Hill, 1990.
11. S.H. Maron, C.F. Prutton, Principles of Physical Chemistry, Mcmillan, 1960.
12. W.J. Moore, Basic Physical Chemistry, Prentice Hall, 1986.

CHEC – 403.1: CHEMISTRY OF ADVANCED MATERIALS

Unit - I: Preparative Techniques

Principle of solid state reactions with reference to MgO and Al₂O₃ - Reaction conditions – Structural considerations – reaction rates – Wagner mechanism – nucleation and diffusion – surface structure and reactivity. Synthesis of MgAl₂O₄ (a spinel) – experimental procedure. Synthesis of a Zeolite - (Na_x(AlO₂)_x(SiO₂)_y)mH₂O - Preparation of thin films – chemical vapour deposition – cathode sputtering – Preparation of metastable phase by sol-gel technique – Hydrothermal technique – Zone melting – Melts – vapour phase transport methods – vapour deposition

Unit - II: Phase Transitions

Buerger's classification – Thermodynamic classification - Ubbelohde's classification – Representation of phase transitions on phase diagrams – Kinetics of phase transitions – Nucleation rate – Avrami equation – Factors that affect the kinetics of phase transitions – crystal chemistry and phase transitions – Martensitic transformations – order-disorder transitions

Unit - III: Chemistry of Selective Materials

Glasses – Oxide glasses – bond type – Viscosity - Zachariasen's rules – Sun-Rowson criterion – Chalcogenide glass – the photocopying process – glass ceramics – applications – refractories – applications.

Solid electrolytes: AgI, RhAg₄I₅, β-Alumina – NASICON – Principles and Applications of solid electrolytes

Ferroelectric, piezoelectric and pyroelectric materials – principle, properties and applications. LED – principle – types – advantages and disadvantages of LED displays

Liquid crystal display LCD – properties – twisted nematic field display – Advantages and disadvantages of LCD – comparison of LCD & LED.

Shape Memory alloys (SMA) – classification – working principles. Non-linear optical materials – second harmonic generators

Unit - IV: Characterization of Nanomaterials

Electron microscopies – scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning Transmission Electron Microscopy (STEM), Scanning Probe Microscopy (SPM) – scanning tunneling microscopy (STM) – Atomic manipulations, Focused Ion beam (FIB) technique – Atomic force microscopy (AFM) – scanning probe Lithography (SPL), Dip pen nanolithography (DPN) - Optical microscopies for nanoscience and Technology – Confocal microscopy – scanning near-field optical microscopy – particle size analysis.

Unit - V: Synthesis and Applications of Nanomaterials

Preparation of nanomaterials – plasma arcing, CVD, electrodeposition, sol-gel synthesis, ball milling, use of natural nanoparticles.

Self assembled monolayers – monolayers on gold – preparation – structure – growth process – patterning monolayers – mixed monolayers – Applications – different types of sensors.

Semiconductor quantum dots – synthesis – electronic structure & spectral properties

Monolayer-protected metal nanoparticles – characterization – functionalization – Application
- Core-Shell nanoparticles – introduction – types of systems – characterization – properties – Applications

Nanosensors – electrochemical sensors, sensors based on physical properties - nanobiosensors

References

1. Anthony R. West, Solid State Chemistry and its Applications, John Wiley, New Delhi, 2007.
2. M. Arumugam, Materials Science, Anuradha Agencies, Kumbakonam (Chapters V and VI) 2nd Edition, 2003.
3. Douglas A. Skoog, F. James Holler, Timothy A. Nieman, Principles of Instrumental Analysis, Saunders, 1998.
4. T. Pradeep, Nano: The Essentials, Tata McGraw Hill, 2007.
5. Mick Wilson, Kamali Kannangara, Geoff Smith, Michelle Simmons, Burkhard Raguse, Nanotechnology, Overseas Press, 2005.

CHEC 403.2: ADVANCED INORGANIC CHEMISTRY

Unit – I Inorganic Reaction Mechanisms - I

Basic principles – Lability, inertness, stability and instability of coordination compounds – substitution reactions of octahedral complexes – Nature of substitution reactions – Theoretical approach to substitution mechanisms – Mechanism of substitution reaction of complexes of cobalt – acid hydrolysis and base hydrolysis of Co(III) complexes.

Unit - II Inorganic Reaction Mechanisms - II

Substitution reactions of square planar complexes – reaction of Pt(II) complexes – trans effect – theories of trans effect – Mechanism of substitution - kinetics of substitution of Pt(II) complexes.

Electron tunneling hypothesis – Marcus – Hush theory – Atom transfer reaction – one electron and two-electron transfer – Inner sphere and outer sphere mechanisms.

Unit - III Chemistry Of Inorganic Materials

Glassy state, glass formers and glass modifiers, applications, ceramic structures, mechanical properties, clay products. Refractories – characterisation properties and applications. Microscopic composites; dispersion strengthened and particle – reinforced, fibre-reinforced composites, macroscopic composites. Nanocrystalline phase, preparation procedures, special properties and applications.

Unit - IV Chemistry of Non-Transition Elements

Peroxo compounds of boron, carbon and sulphur – synthesis, properties and structures of boranes, carboranes, borazines, silicates, silicones - carbides – phosphazenes – sulphur - nitrogen compounds. Interhalogens – pseudohalides and noble gas compounds. Inorganic polymers: Types of inorganic polymers – Metal clusters – Iso and heteropoly acids – polyhalides.

Unit - V Spectral and Magnetic Properties of Complexes

Term state for d ions in Octahedral complexes. Characteristics of d-d transitions. Energy level diagrams of Orgel, Tanabe-Sugano, weak field and strong field concepts. Effect of Jahn Teller distortion, Nephelauxetic effect, Selected examples of d-d spectra – $[\text{Ti}(\text{H}_2\text{O})_6]^{3+}$, trans – $[\text{Cr}(\text{en})_2\text{F}_2]^+$, $[\text{Ni}(\text{en})_3]^{2+}$, $[\text{CoF}_6]^{3-}$, $[\text{Co}(\text{ox})_3]^{3-}$, $[\text{Cu}(\text{H}_2\text{O})_6]^{2+}$.

Magnetism: dia, para – ferro and antiferro – magnetism – quenching of orbital angular momentum, Temp independent paramagnetism – Effect of spin orbit coupling on spectral and magnetic properties.

Text books and References:

1. D.K. Chakraborty, Solid State Chemistry, New Age International, 2010.
2. H.V. Keer, Principles of the Solid State, Wiley Eastern, 1971.
3. H.J. Emeleus, A.G. Sharp, Modern Inorganic Chemistry, ELBS Publication, 1973.
4. J.E. Huheey, Inorganic Chemistry, Addison Wesley, 1993
5. S.F.A. Kettle, Coordination Compounds, Published by Thomas Nelson, 1969.
6. F.A. Cotton, G. Wilkinson, Advanced Inorganic Chemistry, Wiley Eastern, 1988
7. F. Basalo, R.G. Pearson, Mechanism of Inorganic Reactions, Wiley Eastern Publication, 1967
8. M.L. Tobe, Inorganic Reaction Mechanism, Published by Nelson, 1972
9. J.C. Anderson, K.D. Leaver, R.D. Rawlings, J.M. Alexander, Materials Science, 4th Edition, ELBS, Chapman and Hall, 1990.

CHEC 404.1: APPLIED CHEMISTRY

Unit - I: High Polymers

Naturally occurring Polymers— Silk, Wool and collagen
Synthesis, Properties and uses of the following polymers. PE, PP, PVC, PTFE, PMMA, PS, Bakelite, nylons, polyesters, polyamides, polyureas, Synthetic rubbers
Catenanes – 34 Carbon acyloin. Ion Exchange Resins.

Unit - II: Analysis of Water Pollution

Origin of waste water, types, water pollutants and their effects. Sources of water pollution – domestic, industrial, agricultural soil and radioactive wastes as source of pollution, objectives of analysis – parameter for analysis – colour, turbidity, total solids, conductivity, acidity, alkalinity, hardness, chloride, sulphate, fluoride, silica, phosphates and different forms of nitrogen, Heavy metal pollution. Public health significance of cadmium, chromium, copper, lead, zinc, manganese, mercury and arsenic. General survey of instrumental technique for the analysis of heavy metals in aqueous systems. Measurement of DO, BOD and COD. Pesticides as water pollutants and analysis. Water pollution laws and standard.

Unit - III: Applied Photochemistry

Photographic sensitizers – cyanins – pinacyanine, Kryptocyanine – ultraviolet screening agents – Uvinol, Tinuvin – Fluorescent whitening agent – Blankophor– β calcofluor – SD color photography. Additive and subtractive processes. Chemistry of color Developers Flash photolysis. Chemistry of vision – organic transistors - Introduction examples, organic light emitting diodes – Applications

Unit - IV: Fuel Analysis and Agricultural Chemistry

Solid, liquid and gaseous fuels – ultimate and proximate analysis – calorific values – grading of coal – Liquid fuels – flash point, aniline point, octane number and carbon residues. Gaseous fuels - producer gas and water gas.

Analysis of soil: moisture, pH, total nitrogen, phosphorous, silica, lime, magnesia, manganese, sulphur and alkali salts.

Fertilizers: Fertilizer industries in India, manufacture of ammonia, ammonium salts, urea, nitrates, phosphates and superphosphates – mixed fertilizers – nitrogen fixation.

Unit - V: Organic Nanomaterials

Fullerenes – synthesis and purification – magnetic and optical properties. Carbon nanotubes – synthesis purification and functionalization.

Nanosensors – nanoscale organisation for sensors – Self-assembly-template method- biological assembling – Lithographic techniques – molecular nanomachines – introduction – single molecular devices

Text Books and References

1. Stuart Warren, Designing Organic Synthesis, John Wiley & Sons, 1979
2. John D. Roberts, Marjorie C. Caserio, Basic Principles of Organic Chemistry, 2nd Edition, W. A. Benjamin Inc., 1982
3. Charles H. Depuy, Dennis Chapman, Molecular Reactions and Photochemistry, Prentice Hall, 1985
4. W. Carruthers, Some Modern Methods in Organic Synthesis, Cambridge University Press, 1971
5. Burger's Medicinal Chemistry and Drug Discovery, Vol. I. Edited by Donald J. Abraham, John Wiley & Sons, 2nd edition, 2003.
6. T. Pradeep, Nano: The Essentials", Tata McGraw Hill, 2007.
7. M.L. Jackson, Soil Chemical Analysis, Prentice Hall of India, 1973
8. S.M. Khopkar, Environmental Pollution Analysis, New Age International, 2nd edition, 2011.
9. S.S. Dara, A Text Book of Environmental Chemistry and Pollution Control, S.Chand & Company Ltd., 1993.

CHEC 404.2: INDUSTRIAL AND MEDICINAL CHEMISTRY (Revised with effect from 2014)

Unit - I Green Chemistry

Introduction and principle of green chemistry - Environmental friendly green techniques - solvent supported catalysts and reagents, heterogenous reactions, Examples for organic reactions involving green chemistry techniques.

Unit - II Supramolecular Chemistry

Definition of Supramolecular Chemistry, Nature of binding interactions in supramolecular structure: ion-ion, ion-dipole, dipole-dipole, H-bonding, cation-p, anion-p, p-p, and Van der Waals interaction.

Synthesis of crown ethers, cryptands, calixarenes, cyclodextrins, cyclophanes, cryptophanes and dendrimers.

Unit - III Introduction to Computational Chemistry

An introduction to concepts of potential energy surface, Basic principles of molecular mechanics, Basic principles of Ab initio method - Basics principles of Semiempirical calculations (SE) - Basics principles of Density functional theory (DFT). Softwares.

Unit - IV Drug Design

Development of new drugs, Procedures followed in drug design. Structure Activity Relationship (SAR) of morphines and Penicillins. Physico – chemical parameters: Lipophilicity, partition coefficient, electronic ionization constants, Quantitative Structure Activity Relationship. Free – Wilson analysis, Hansch analysis, relationships between – Wilson and Hansch analysis – case study. Concepts of drug receptors. Elementary treatment of Drug receptor interactions.

Unit - V Drug Synthesis

Synthesis of the following drugs

- a. Anxiolytics – Benzodiazepines
- b. Neuroleptics – Phenothiazines
- c. Hypnotics and Sedatives – Piperidinediones
- d. Local anesthetics – Aminobenzoic acid and its derivatives
- e. Anti – coagulants – 1,3 – Indanedione derivatives
- f. Hypoglycemic agents – Sulfonylureas
- g. Antihistaminic agents – Ethylenediamine derivatives
- h. Antimalarials – Aminoquinolines
- i. Analgesics and Antipyretics – Paracetamol, Phenylbutazone.
- j. Anti – inflammatory – Diclofenac

References

1. Rashmi Sanghi, M.M.Srivastava, Green Chemistry: Environment Friendly Alternatives, Narosa Publishers, 2003
2. J.M. Lehn, Supramolecular Chemistry – Concepts & Perspectives, Wiley VCH, 1995
3. P. D. Beer, P.A. Gale, D.K. Smith, Supramolecular Chemistry, Oxford University Press, 1999
4. J.W. Steed, J.L. Atwood, Supramolecular Chemistry, John Wiley Sons, 2000
5. Errol G. Lewars, Computational Chemistry (Introduction to Theory and Applications of Molecular and Quantum Mechanics), Springer, 2003
6. Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical Chemistry, Ed. Robert F. Doerge, 2 011.
7. Graham L. Patrick, An Introduction to Medicinal Chemistry, Oxford, 2009
8. K.Ilango, P.Valentina, Text Book of Medicinal Chemistry, Vol. I, Kreethi Publishers, 2007
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CHEP 405: ORGANIC PRACTICAL – II

- I. Preparation of Organic compounds involving two stages.
- II. Quantitative analysis and Estimation of phenol, aniline, methyl ketone and glucose by volumetric analysis

CHEP 406: INORGANIC PRACTICAL – II

I. Quantitative analysis

- 1) Estimation of Ba²⁺ and Ca²⁺ ions
- 2) Estimation of Cu²⁺ and Ni²⁺ ions
- 3) Estimation of Cu²⁺ and Zn²⁺ ions
- 4) Estimation of Cu²⁺ and SO₄²⁻ ions
- 5) Estimation of Ca²⁺ and Mg²⁺ ions
- 6) Analysis of pyrolusite

II Preparation of the following Inorganic complexes

- 1) Tris (thiourea) copper(I) chloride
- 2) Potassium trioxalatoferrate
- 3) Tetraammine copper(II) sulphate
- 4) Microcosmic salt
- 5) Chrome alum
- 6) Trans-Diaquadioxalatochromate(III)

CHEP 407: PHYSICAL CHEMISTRY PRACTICAL – II

I. Potentiometry

- 1) Single electrode potentials
- 2) Solubility of sparingly soluble salt
- 3) Ratiometric titrations
 - i) Redox titrations
 - a) Ferrous iron (II) **vs.** dichromate (Fe^{2+} **vs.** $\text{Cr}_2\text{O}_7^{2-}$)
 - b) Iodide ion (I^-) **vs.** KMnO_4
 - c) Ferrous iron (II) **vs.** Cerium (IV) ion (Fe^{2+} **vs.** Ce^{4+})
 - ii) Precipitation titrations
 - a) Chloride Vs. Silver ion, b) Iodide Vs. Silver ion,
 - c) Mixture of chloride and iodide ion Vs. Silver ion
- 5) Potentiometric titrations (by quinhydrone electrode)
 - a) Strong acid **vs** Strong base
 - b) Dissociation constant of a weak acid vs NaOH
 - c) Mixture of acids (HCl, CH_3COOH) **vs** NaOH

II. Polarimetry

- 1) Determination of Specific Rotation
- 2) Inversion of Sucrose

III. Chemical Kinetics

- 1) Acid catalysed hydrolysis of an ester.
- 2) Comparison of acid strengths.
- 3) Persulphate – iodide kinetics – clock reaction – Primary salt effects
- 4) Influence of Cu^{2+} and Fe^{3+} on the reaction between persulphate and iodide ions.

IV. pH Metry

- 1) Dissociation constant of dibasic acid