M. Sc., Chemistry Syllabus for year 2019-20

Programme Educational Objectives (PEO)

- To impart higher level of theoretical and practical knowledge thorough understanding in frontier areas of chemistry
- To make the students to pursue advanced studies and continue research in frontier fields of chemistry and competent enough to tackle complex multifaceted problems in research and industries.
- To develop the skills and knowledge needed for the real life situations and face competitive examinations and interview with confidence.

Programme Specific Outcomes (PSO)

After completion of the programme, the students will be able to

- Perform as responsible individual with ethical values and accountable to the society.
- Apply the knowledge and concepts in needed situations, i.e., in industries, research, and academic.
- Endure competitive examinations and interviews with confidence.
- Execute their technical skills to handle standard equipment's and to interpret the data.

SCHEME OF EXAMINATION

SEMESTER–I								
S.No.	Course Code	Course Title	Hrs/ wk	Credits	Exm. Hrs	Max. Marks		
						Int	Ext	Tot
1	13PCH1C01	Core: Inorganic Chemistry–I (Nuclear and Solid State Chemistry)	5	5	3	25	75	100
2	13PCH1C02	Core: Organic Chemistry–I (Organic Reaction Mechanism–I)	5	4	3	25	75	100
3	13PCH1C03	Core: Physical Methods in Chemistry (Group Theory and Spectroscopy)	5	4	3	25	75	100
4	19PCH1EL1	Elective: Analytical Chemistry	5	4	3	25	75	100
5	15PCH2CP1	Core Practical: Inorganic Chemistry–I	3	–	–	–	–	–
6	15PCH2CP2	Core Practical: Organic Chemistry–I	3	–	–	–	–	–
7	15PCH2CP3	Core Practical: Physical Chemistry–I	4	–	–	–	–	–
		Subtotal–I	30	**17**				**400**

SEMESTER–II								
S.No.	Course Code	Course Title	Hrs/ wk	Credits	Exm. Hrs	Max. Marks		
						Int	Ext	Tot
1	13PCH2C04	Core: Inorganic Chemistry–II (Coordination Chemistry)	5	5	3	25	75	100
2	13PCH205	Core: Organic Chemistry–II (Organic Reaction Mechanism–II)	5	4	3	25	75	100
3	13PCH2C06	Core: Physical Chemistry–I (Quantum Chemistry & Spectroscopy)	5	4	3	25	75	100
4	13PCH2EL2	Elective: Polymer Chemistry	5	4	3	25	75	100
5	15PCH2CP1	Core Practical: Inorganic Chemistry–I	3	3	6	40	60	100
6	15PCH2CP2	Core Practical: Organic Chemistry–I	3	3	6	40	60	100
7	15PCH2CP3	Core Practical: Physical Chemistry–I	4	3	6	40	60	100
		Subtotal–II	30	**26**				**700**

SEMESTER - III								
S. No.	**Course Code**	**Course Title**	**Hrs/ wk**	**Credits**	**Exm. Hrs**	**Max. Marks**		
						Int	**Ext**	**Tot**
1	13PCH3C0O7	Core: Physical Chemistry–II (Thermodynamics)	5	5	3	25	75	100
2	13PCH3C08	Core: Organic Chemistry–III (Chemistry of Natural Products)	5	5	3	25	75	100
3	19PCH3C09	Core: Computational Chemistry and Molecular Modelling	5	4	3	25	75	100
4	13PCH3EL3	Elective: Organic Reactions and Reagents	5	4	3	25	75	100
5	15PCH4CP4	Core Practical: Inorganic Chemistry–II	3	–	–	–	–	–
6	15PCH4CP5	Core Practical: Organic Chemistry–II	3	–	–	–	–	–
7	15PCH4CP6	Core Practical: Physical Chemistry–II	4	–	–	–	–	–
		Subtotal–III	30	18				**400**

SEMESTER–IV								
S. No.	**Course Code**	**Course Title**	**Hrs/ wk**	**Credits**	**Exm. Hrs**	**Max. Marks**		
						Int	**Ext**	**Tot**
1	13PCH4C10	Core: Physical Chemistry–III (Chemical Kinetics & Electrochemistry)	5	5	3	25	75	100
2	17PCH4EL4	Elective: Green and NanoChemistry	5	4	3	25	75	100
3	17PCH4EL5	Elective: Medicinal Chemistry	5	5	3	25	75	100
4	13PCH4PRO	Core: Project Work and Viva Voce[$]	5	5	–	–	100	100
5	13PCH4CP4	Core Practical: Inorganic Chemistry–II	3	3	6	40	60	100
6	13PCH4CP5	Core Practical: Organic Chemistry–II	3	3	6	40	60	100
7	13PCH4CP6	Core Practical: Physical Chemistry–II	4	4	6	40	60	100
		Subtotal–IV	30	**29**				**700**
GRAND TOTAL				**90**				**2200**

[$]Project Work &Viva Voce=**100** marks [Dissertation: **60** marks& Viva voce:**40** marks)

Programme: M.Sc., Chemistry Course Code: 13PCH1C01
CORE: Inorganic Chemistry–I
(Nuclear and Solid State Chemistry)
Year: I Semester: I Credits: 5 Total Hours: 5 x15 = 75

UNIT–I

Nuclear models: the shell model–the liquid drop model. Units of radioactivity.Alpha decay–range, ionizing power, energy spectrum, Geiger–Nutta's rule, theories of alpha decay–tunnel effect. Beta decay–types–$\beta^-$and β^+ decay, electron capture, absorption, range and energy. Gamma ray–radiative de–excitation, decay constant, nuclear isomerism, internal conversion, the Auger effect.Artificial radioactivity.

Detection and measurement of radioactivity–proportional counter, G.M. counter, scintillation counter, semiconductor detector, cloud chamber and bubble chamber.

UNIT–II

Nuclear reactions: Bethe's notation. Scattering, photonuclear, evaporation, spallation, fission, fragmentation, stripping and pick–up reactions.Reaction cross section, Q value, threshold energy, and columbic barrier. Nuclear reactions induced by neutrons and protons. Charged particle accelerators–linearaccelerator, cyclotron, beatatron and bevatron.Types of fission reactions.

UNIT–III

Nuclear energy sources: nuclear fission energy & nuclear reactors, the four factor formula–Classification of reactors–thermal, natural uranium, heavy water, heterogeneous water cooled and PHWR. Critical size of a thermal reactor–Fast Breeder reactor.Energy from nuclear fusion–Stellar energy–thermonuclear reactions on earth–fusion bomb. Applications of radioactive isotopes as tracers, chemical investigations, analytical applications–isotopic dilution, neutron activation–radiometric titration, Libby's C–14 dating method–industrial and medical applications.

UNIT–IV

Solid state chemistry: Ionic crystals–coordination number, radius ratio rule and shapes of ionic crystals–structures of ionic crystals–AX type CsCl, ZnS (Zinc blende and Wurtzite)–AX_2 type calcium fluoride, titanium dioxide, cadmium iodide. Experimental methods of crystal structure determination–X–ray diffraction, electron diffraction and neutron diffraction. Comparative study of the three diffraction methods.

UNIT–V

Inorganic polymers:preparation, structure, reactions and uses of silicone polymers, silicone fluids, gums, elastomers and resins. Phosphonitrilic compounds–trimer and tetramer. Nitrides of sulphur–S_4N_4, $(NSF)_3$, $(NSF)_4$. Isopoly and heteropoly acids of molybdenum and tungsten–preparation, reactions, uses and structures–boranes–Wade's rule–calculation of frame work electrons.

Reference Books

1. H.J. Arnikar, Essential of Nuclear chemistry, New Age International Publishers,

Edn.4 (1997).

2. U. N. Dash, Nuclear Chemistry, Edn. 1 (1971)

3. GurudeepRaj, Advanced Inorganic Chemistry, Vol. I,KrishnaPrakasam Media (P) Ltd., Edn. 25 (1999).
4. B.R. Puri, L.R Sharma and K.C. Kalia, Principles of Inorganic chemistry, Vallabh Publishers (2005).

Programme: M.Sc., Chemistry Course Code: 13PCH1C02
CORE: Organic Chemistry–I*(Organic Reaction Mechanism–I)*
Year: I Semester: I Credits: 4 Total Hours: 5 x15 = 75

UNIT-I

Aromaticity – Benzenoid and non-benzenoid aromatics - ferrocene, azulene and annulenes. Alternant and non-alternant hydrocarbons – homoaromaticity – antiaromaticity. Kinetic and non-kinetic methods of study of reaction mechanisms – primary kinetic isotopic effect, study of intermediates, isotopic labelling and cross over experiments. Hammond's postulates. Linear free energy relationship – Hammet equation.

UNIT-II

Arenium ion mechanism – orientation and reactivity of mono and disubstituted benzenes. Aromatic electrophilic substitution reactions. Formylation-Gattermann, Gattermann Koch, Reimer-Tiemann, Kolbe, Bischler-Napieralski, Hoffmann - Maritus and Jacobsons reactions. Friedel-Crafts alkylation and acylation. Aromatic nucleophilic substitution reactions-Benzyne mechanism-Intermediate complex mechanism and S_NAr mechanism-structure reactivity relationship-Ziegler alkylation and Chichibabin reaction.

UNIT-III

Aliphatic nucleophilic substitution reactions- S_N1, S_N2, S_Ni, S_N1', S_N2' and S_Ni' mechanisms, substitution at vinyl carbon-stereochemistry of nucleophilic substitution reaction-effect of substrate structure-solvent effect-leaving group effect-nucleophilicity-ambident nucleophiles and ambident substrates, neighboring group participation. Aliphatic electrophilic substitution reactions-SE_1, SE_2 andSE_i mechanisms, structure reactivity relationship. Friedel Crafts acylation at olefinic carbon – Stork – enamine reaction.

UNIT-IV

Electrophilic, nucleophilic and free radical addition reaction to double and triple bonds-Hydration, hydroboration, Michael addition, epoxidation and hydroxylation. Addition reactions to carbonyl compounds-Mannich reaction-Meerwein Ponndorff – Verley (MPV) reduction-addition of Grignard reagents to aldehydes and ketones-Claisen, Dieckmann, Stobbe, Knoevenagel, Darzen, Wittig, Thorpe and Benzoin reactions.

UNIT-V

Elimination reactions: E1, E2, Ei, $E1_cB$ mechanisms, stereochemistry of elimination reactions, effect of substrate structure, effect of attacking base, effect of leaving group, effect of medium and eliminations vs substitution. Typical elimination reactions-Chugaev reaction, Hoffmann degradation, Cope elimination and dehydration of alcohols. Carbenes and nitrenes-structure, generation and reactions.

Text &Reference Books

1. Jerry March, Advanced Organic Chemistry, (Reaction Mechanism and structure). McGraw Hill Gogakusha, New Delhi (1977)
2. I. L. Finar Organic Chemistry, ELBS, Edn V (1975)
3. R. L. Morrision and R. N. Boyd, Organic Chemistry,Prentice Hall of India Pvt Ltd, Edn. VI (1992).
4. Badger, Aromaticity and Aromatic Character,Cambridge University Press (1969)
5. Petersykes Guide book to mechanisms in Organic Chemistry,OrientLongmann (1986)
6. Jagadamba Singh and L.D.S.Yadav, Advanced Organic Chemistry, PragatiPrakashan (2004).

Programme: M.Sc. Chemistry Course Code: 13PCH1C03
CORE: Physical Methods in Chemistry
(Group theory and spectroscopy)
Year: I Semester: I Credits: 4 Total Hours: 5 x15 = 75

UNIT - I

Symmetry elements and symmetry operations. Inverse operations. Definition of a group-properties of a group, definition of abelian group, cyclic group, finite group, infinite group, sub-group and isomorphic group-group multiplication tables. Symmetry classification of molecules into point groups (Schoenflies symbols only).

Matrices: Definition of matrix, diagonal matrix, null matrix, unit matrix, row matrix, column matrix, symmetric matrix, skew matrix and conjugate matrix. Matrix multiplication. Determination of inverse matrix. Block multiplication of matrices. Matrix notations of symmetry operations of C2V and C3V point groups.

UNIT – II

Definition of reducible and irreducible representations. Direct product rule. The great orthogonality theorem and its consequences (statement only proof not needed). Construction of character table for C_2V & C_3V point groups. Calculation of character values of reducible representation per unshifted atom for each type of symmetry operation. Determination of total Cartesian representation.

Group Theory and Vibrational Spectroscopy: Vibrational modes as bases for group representations. Symmetry selection rules for IR and Raman spectra(mutual exclusion principle). Classifications of vibrational modes.

Applications of group theory to bonding: Hybridization schemes for orbitals in AB3(planar).AB_4(Td), AB5(D_3h), AB_6(Oh) types of molecules. Hybridization schemes for bonding in AB_3(D_3h) and AB_6(Oh) types of molecules. Group theory and dipole moment.

UNIT – III

IR Spectroscopy – Theory - IR region. Molecular vibrations – calculation ofvibrational frequency. Number of fundamental vibrations – selection rules – factors influencing vibrational frequencies – instrumentation – Finger print region–identification of functional groups–application of IR spectroscopy to simple organic molecules. The Raman effect – Stoke's and antistoke's lines. Comparison between IR and Raman spectra.

UNIT – IV

Ultraviolet and visible spectroscopy Theory, Beer and Lambert's laws. Types of electronic transitions-selection rules-Franck-Condon principle. Born-Oppenheimer Approximation. Designation of bands(R, K and B bands) Chromophores and auxochromes. Bathochromic, hypsochromic, hyperchromic and hypochromic shifts.

photometric titrations. Woodward- Fieser rules for calculating absorption maximum of dienes, polyenes and α, β-unsaturated carbonyl compounds.

UNIT – V

Mass Spectrometry-Presentation of mass spectrum-instrumentation-sample insertion, ion source, mass analyzer and ion detectors. Resolution.Types of ions-molecular ion, fragment ion, rearrangement ion, metastable ion, odd and even electron ions. Molecular ion peak, base peak and metastable ion peak. Nitrogen Rule, Isotope abundances. Fragmentation of aldehydes and ketones, alcohols, phenols, carboxylic acids and amines. Retro-Diels Alder Reaction. McLafferty rearrangement. Double bond and ring equivalence.

Text & Reference Books

1. F.A. Cotton, Chemical applications of group theory, Wiley Eastern Ltd Edn. 2, (1988).
2. R.M. Silverstein, G. Clayton Bassler, and Terence C. Morril, Spectrophotometric identification of organic compounds. John Wiley & sons Edn. 5. (1991).
3. F. Sheinmann, An introduction to spectroscopic methods for identification of organic compounds, Vol. I & II by, Pergamon Press(1970)
4. C.K. Banwell,Fundamentals of molecular spectroscopy, Tata McGraw Hill(1983).
5. W. Kemp Organic Spectroscopic, ELBS, Edn.3 (1991).
6. Das and James,Organic Mass Spectroscopy, Oxford GBH Publishing, New Delhi (1976).
7. P.S. Kalsi, Spectroscopy of organic compounds, Wiley Eastern Ltd.
8. Jag Mohan, Organic Spectroscopy–principles and applications II Edition Narosa Publishing House Pvt. Ltd.
9. K.Veera Reddy, Symmetry and Spectroscopy of molecules, New Age International (1998).
10. Y. R. Sharma, Elementary organic spectroscopy, S. Chand & Co (2007)

Programme: M.Sc. Chemistry Course Code: 19PCH1EL1
Elective I: **Analytical Chemistry**
Year: I Semester: I Credits: 4 Total Hours: 5 x 15 = 75

UNIT – I

Thermal methods of analysis: principle, instrumentation and applications of thermogravimetry, differential thermal analysis and differential scanning calorimetry, - thermometric titrations. Refractometry- theory, Abbe's refractometer and applications of refractometry.

UNIT – II

Polarimetry – Plane polarised light – optical activity of molecules – polarimeter and its uses. ORD and CD spectrometry, circular birefringence, circular dichroism , optical rotatory dispersion , plain curves , anomalous curves - Cotton effect – axial haloketone rule and octant rule – application.Nephelometry and Trubidimetry-principle, instrumentation and applications.

UNIT – III

Atomic Absorption Spectrometry: principle- instrumentation – detection of metals & non-metals, interference, detection limit & sensitivity and applications.
Flame Emission spectrometry- Principle, instrumentation, methodology and applications. Comparison between AAS and FES.
Molecular fluorescence and phosphorescence-Theory, instrumentation and applications.

UNIT-IV

Chromatographic methods: Basic principles, theories, instrumentation, experimental procedures and application of following chromatographic techniques – paper , thin layer , column , gas chromatography, high performance liquid chromatography and ion-exchange chromatography.

UNIT – V

Significant figures, errors – determinate and indeterminate, precision, mean, median, mode, average deviation, standard deviation (sample and population) - relative standard deviation – accuracy, difference between precision and accuracy, propagation of determinate errors, reporting of analytical data- uncertainty, statistical treatment of analytical data-Confidence limits, Student's t-values for various probability levels and varying degrees of freedom. Rejection of a result-Q-test, tests of significance – F-test and t-test.

References

1. B.K. Sharma, Chromatography , Goel Publishing House.(2004)
2. Gurdeep R. Chatwal& S.K. Anand, Instrumental Methods of Chemical Analysis, Himalaya Publishing House (2003) .
3. B.K. Sharma, Instrumental Methods of Chemical Analysis, Goel Publishing House (2003).
4. D. Nasipuri, Stereochemistry of Organic Compounds, New Age International Publishers.(2010).
5. B.R.Puri, L.R. Sharma and K.C.Kalia, Principles of Inorganic Chemistry, Milestone Publishers (2010).
6. Larry G.Hargis, Analytical chemistry, Prentice Hall(1988).

Programme: M.Sc. Chemistry Course Code: 13PCH2C04
CORE: Inorganic Chemistry–II*(Coordination Chemistry)*
Year: I Semester: II Credits: 5 Total Hours: 5 x15 = 75

UNIT–I

Bonding in coordination complexes: Crystal field theory (CFT) – crystal field splitting in octahedral, tetrahedral and square planar complexes, factors affecting crystal field stabilization energy (CFSE) – spectrochemical series – magnetic and spectral properties, colours of transition metal complexes – applications of CFSE. Molecular orbital Theory (MOT)-MO diagrams of octahedral, tetrahedral and square planar symmetries. Experimental evidences for pi-bonding.

UNIT –II

Electronic spectra of transition metal complexes: Derivation of Term symbols to P^2 and d^2, spin-spin and spin orbit couplings-selection rules and relaxations- splitting of electronic energy levels and spectroscopic states- Orgel Diagram- interpretation of electronic spectra of d^1 to d^9 metal ions- Tanabe – Sugano diagrams of d^2 and d^3 systems. Jahn – Teller tetragonal distortions- Nephelauxetic effect. Charge transfer spectra.

UNIT – III

Chemistry of pi-acceptor ligand complexes: Preparative methods, reactions, structure and bonding of transition metal carbonyls, carbonyl hydrides, carbonyl halides, nitrosyls, and dinitrogen complexes. Applications of IR spectroscopy to metal carbonyls. Organometallic compounds: preparation, structure and bonding in metal – alkenes, alkyne, allyl and butadiene complexes. Metallocenes: preparation, properties and bonding in ferrocene. Preparation and structure of arene complexes formed by seven and eight membered rings.

Unit – IV

Complexes of biochemical importance: structure and functions of Cytochromes, Myoglobin and Hemoglobin, Ferredoxins, Chlorophyll and Cyanocobalamin (Vitamin B12).
Ligand substitution reactions in octahedral complexes: Types of substitution reactions – mechanism of S_N1 and S_N2 reactions, acid and base hydrolysis reactions - S_N1_{CB} mechanism. Anation reactions.

UNIT – V

Ligand substitution reactions in square-planar complexes: Trans effect-theories of trans effect, applications of trans effect-mechanism of substitution reactions in square-planar complexes. Complementary electron transfer reactions. Catalysis by organometallic compounds - alkene hydrogenation (Wilkinson's catalyst), hydroformylation(oxo proces), Monsanto acetic acid process, the Wacker process and Ziegler –Natta catalysis.

References

1. J.E. Huheey, E.A. Keither and R.L. Keither, Inorganic chemistry, Harper Collins College Publishers, Edn 4(1993).
2. J.D. Lee, Concise Inorganic chemistry, Blackwell science Edn. 2 (1996).
3. W.U. Malik, G.D.Tuli and R.D. Madan, Selected Topics in Inorganic Chemistry, S.Chand& Co. (2004).
4. Gurdeep Raj, Advanced Inorganic Chemistry Vol–II, Goel Publishing House (2004).
5. F.A. Cotton and G. Wilkenson, Advanced Inorganic Chemistry Wiley & Sons.Edn.6 (2006).
6. H.J. Emeleus and A.G. Sharpe Modern Aspects of Inorganic Chemistry, ELBSEdn. 4 (1973).

Programme: M.Sc. Chemistry Course Code: 13PCH2C05
CORE: Organic Chemistry–II*(Organic Reaction Mechanism –II)*
Year: I Semester: II Credits: 4 Total Hours: 5 x 15 = 75

UNIT-I

Pericyclic reactions: Electrocyclic reactions - molecular orbital correlation diagram and frontier molecular orbital (FMO) theory applicable to the electrocyclic conversion of 1,3 – dienes and 1,3,5 – trienes, [2+2] cycloadditions and [2+4] cycloadditions. Sigmatropic rearrangements-[1,5] sigmatropic rearrangement, Claisen and Cope rearrangements. The perturbation theory of pericyclic reactions. Di-π-methane rearrangement, ene reactions and 1, 3-dipolar additions.

UNIT-II

Photochemistry: Introductory theory of light absorption-Jablonski diagram, dissipation of excess energy of the excited molecules, radiative transitions – fluorescence, phosphorescence, delayed fluorescence – e – type and p – type. Radiative transitions involving more than one molecule-excimers, exciplexes. Radiationless transitions involving internal conversion and intersystem crossing, energy transfer – intermolecular and intramolecular-photosensitisation and quenching. Photochemical reactions of ketones - Paterno-Buchi reaction, Norrish type type II reactions and cis-trans isomerization, photoreduction and photo oxidation, I.

UNIT-III

Oxidation by chromic acid, manganese (IV) oxide, silver carbonate, dimethyl sulphoxide, dess-Martin periodinane oxidation, Oxidations of carbon-carbon double bonds – epoxides, enantioselective epioxidation of allylic alcohols (sharpless asymmetric epoxidation) – diastereo selective epoxidation of homo allylic alcohols, m-chloroperbenzoic acid and osmium tetroxide, Prevost reaction, catalytic hydrogenation, selectivity of reduction, reduction of functional groups (alkenes, alkynes, aldehydes and ketones), stereochemistry and mechanism, homogeneous hydrogenation.

Reduction by dissolving metals-metal and acid, metal and alcohol. Reduction by hydride transfer reagents – di-isobutyl aluminium hydride (DIBAL-H), alkoxy, alkyl and acyloxy borohydrides. Metal catalysed Carbon – Carbon bond forming reaction – Suzuki and Hech coupling.

UNIT-IV

Acids and Bases: Arrhenius theory, Bronsted theory, acidic and basic solvents, levelling effect, measurement of solvent acidity, acid and base catalysis, Lewis acids and bases. Effect of structure on strength of acids and bases-inductive effect-resonance effect-state of hybridization. Effect of medium on acid and base strength. Hard and soft acids and bases. HSAB Principle-MO theory and applications of HSAB theory.

UNIT-V

Conformational analysis and stereochemistry: Conformations of cyclohexane, substituted cyclohexanes and decalins. Conformation and reactivity in substituted cyclohexanes. Assignment of R and S configuration in chiral non-racemic molecules. Stereochemistry of biphenyls, allenes and spiranes. Stereochemistry of sulphur and nitrogen compounds. Stereochemical reagents in organic reactions- Wilkinson catalyst, t-C_4H_9 COOH, (+)n diethyl tartrate, di-isopropyl tartrate and tetra isopropyltitanium

References

1. Jerry March, Advanced Organic Chemistry (Reaction Mechanism and Structure). McGraw Hill Gogakusha, New Delhi (1977)
2. E. L. Eliel Stereochemistry of Carbon compounds, Tata McGraw Hill (1962)
3. C.H.Depuy and O. C. Chapman, Molecular reactions and Photochemistry, Prentice Hall (1975)
4. S. Muherjee and S. P. Singh, Reaction Mechanisms in Organic Chemistry (1976)
5. R. K. Bansal, Organic reaction mechanisms, Tata McGraw Hill, Edn. 2 (1986)
6. K. Nasipuri, Stereochemistry of Organic Compounds–Principles and applications, Wiley Eastern Limited (1992).
7. W.M.Horspool, Aspects of Organic Photochemistry, Academic Press (1976)
8. Jagadamba Singh, Photochemistry and Pericyclic reactions, New Age Int.Pvt.Ltd. (2003)
9. I.L. Finar, Organic Chemistry Vol–II, Stereochemistry and the Chemistry of Natural Products, ELBS, 5th Edition
10. N. Tewari, Advanced Organic Stereochemistry (Problems and Solutions) (2010)

Programme: M.Sc. Chemistry Course Code:13PCH2C06
CORE: Physical Chemistry–I
(Quantum chemistry and spectroscopy)
Year: I Semester: II Credits: 4 Total Hours: 5 x 15 = 75

UNIT I

Blackbody radiation – failure of classical theories (Wein law and Rayleigh-Jeans law only) Planck's quantum theory in explaining blackbody radiation. Einstein's theory of photoelectric effect.

H-atomic spectrum-de-Broglie hypothesis. Heisenberg's uncertainty principle. Time-dependent and time-independent Schrodinger equations-interpretation of wave function and requirements of wave functions. Operators-addition and subtraction, product of operators, commutator and linear operator. Eigen functions and eigen values. Correspondence between physical quantities and operators. Hamiltonian and angular momentum operators. Postulates of quantum mechanics.

UNIT II

Treatment of particle in one dimensional box-quantization of energy, normalization of wave function, orthogonality of a particle in one dimensional box-illustration of uncertainty principle for a particle in one dimensional box, particle in a three dimensional box-principle of separation of variables. Harmonic oscillator model of a diatomic molecule-finding asymptotic solution of Schrodinger equation for a one-dimensional harmonic oscillator. Rigid rotator model of a diatomic molecule solving the Φ equation of Schrodinger equation of the rigid rotator. H-atom (H like species) (solving radial and θ equations not necessary). Shapes of orbitals.

UNIT III

Electron spin -He-atom- Pauli exclusion principle- anti symmetric wave functions. Approximate wave functions for many electron atoms. Need for approximation methods-perturbation (first order only) and variation methods, applications of perturbation method to He atom, application of variation method to He atom. Born-Oppenheimer approximation-Hamiltonian operator for a hydrogen molecule using Born-Oppenheimer approximation.

UNIT IV

Mossbauer spectroscopy - Principle, Instrumentation, isomer shift, quadruple interaction, nuclear Zeeman splitting and applications.

ESR theory-instrumentation, derivative curves, 'g' shift, hyperfine splitting,isotropic and anisotropic systems, zero field splitting and Kramer's degeneracy, applications of ESR spectroscopy.

UNIT – V

NMR- Spectroscopy-theory – instrumentation – FT NMR, chemical shift – factors influencing chemical shift, chemical and magnetic equivalence – correlation data, influence of restricted rotation, solvents used – spin-spin coupling – factors influencing coupling constant, proton exchange reactions, hetero nuclear coupling – deuterium exchange, simplification of complex spectra – increased field strengths – double resonance – lanthanide shift reagents, applications of NMR to simple organic molecules, 2D NMR – basic concept–COSEY spectrum, C^{13} NMR– double resonance- nuclear Overhauser effect (NOE) –

off resonance decoupling, proton noise decoupling – basic ideas only, comparison between C^{13} and H^{1} NMR.

Reference Books

1. Silverstein, Bassler and Morril Spectroscopy identification of organic compounds, Hohn Wiley.
2. F. Sheinmann An introduction to Spectroscopic methods for the identification of Organic CompoundsVol I &Vol II ,Pergamon Press, Edn. 1 (1973).
3. R.S.Drago Physical methods in inorganic chemistry
4. K. L. Pavia and G. M. Lapmann. Introduction to Spectroscopy .
5. P. S. Kalsi Spectroscopy of organic compounds , Wiley Eastern Ltd (1971).
6. B.K. Sen, Quantum Chemistry including molecular spectroscopy, Tata McGraw Hill Edn(1992).
7. R. K. Prasad,Quantum Chemistry , New Age Publishers(1994).
8. Donald A. McQuarrie, Quantum Chemistry, Oxford University Press.

Programme: M.Sc. Chemistry Course Code: 13PCH2EL2
Elective : **Polymer Chemistry**
Year: I Semester: II Credits: 4 Total Hours: 5 x 15 = 75

UNIT I

Mechanism of Polymerisation– Functionality of monomers, classification of polymers, degree of polymerisation and stereoregularity of polymers-isotactic, syndiotactic and atactic. Polymerisation mechanisms- step and addition (kinetics not required). Ring-opening polymerisation and mechanisms of Ziegler-Natta Polymerisation.

UNIT II

Polymerization Techniques- Bulk, solution, suspension, emulsion, melt condensation and interfacial polycondensation.

Molecular weight and size: number average and weight average molecular weights. Sedimentation and viscosity average molecular weights. Determination of molecular weights.- gel permeation chromatography, end group analysis, viscometry and sedimentation velocity methods.

UNIT III

Thermal properties- glass transition temperature (Tg)- crystalline melting point (Tm)-relationship between Tm and Tg, transitions associated properties-factors affecting Tg-its relationship with molecular weight and melting point. Effects of plasticizers and co-polymerisation on Tg.

Reactions of Polymer-Hydrolysis, hydrogenation and cyclisation reactions. Polymer degradation- Thermal, photo and oxidative degradations.

UNIT IV

Technology of Polymers-Processing techniques-calendering, die casting, rotational casting, film casting, compression, injection, blow and extrusion moulding methods. Fibre technology-textile and fibre properties, spinning, fibre after treatment. Elastomer technology-Natural rubber, chemistry of vulcanization, reinforcement, elastomer properties and compounding.Polymer additives-fillers, plasticisers, antioxidants, colourants, flame-retardants and stabilizers.

UNIT V

Specialty Polymers: Conducting polymers, liquid crystalline polymers, and photopolymers, and electroluminescent polymers, polymers for electronic and biomedical applications. Basics of polymer composites.

Miscellaneous Polymers: Methods of preparation, properties and uses of - Teflon, PMMA, Polyethylene, Polystyrene, PAN, Polyesters, Polycarbonates, Polyamides, Polyurethanes, PVC, Buna rubbers, Neoprene rubbers, Epoxy resins, Phenol - formaldehyde and Urea-formaldehyde resins.

Text & Reference Books

1. V.R Gowariker, N.V. Viswanathan and JayadevSreedhar, Polymer Science, New Age International (2010).
2. F. W. Billmeyer, Text Books of Polymer Science, John Wiley and sons (2003).
3. J. R. Fried, Polymer Science and Technology, Prentice Hall (2003).
4. PremamoyGhosh, Polymer Science and Technology of Plastics and Rubbers, Tata McGraw–Hill (2002).
5. A.L.Gupta, Polymer Chemistry, PragatiPrakashan (2010).

Programme: M.Sc. Chemistry Course Code:15PCH2CP1
Core Practical: Inorganic Chemistry–I
Year: I Semester: I &II Credits: 3 Total Hours: 3 x 30 = 90

A. Semimicro qualitative Analysis of a mixture containing two common and two less common cations like Thallium, Tungsten, Selenium, Tellurium, Molybdenum, Cerium, Thorium, Zirconium, Vanadium, Beryllium and Lithium.

B. Preparation of the inorganic complexesTris(thiourea)copper(II) sulphate dihydrate,Potassium trioxalatochromate(III), Hexathiourealead(II) nitrate, Potassium trioxalatoaluminate(III), Tristhioureacopper(I) chloride.

C. Colorimetric estimations (using photoelectric colorimeter)
Copper, Iron, Nickel, Manganese and Chromium.

References

1. V. V. Ramanujum, Semimicro Qualitative Inorganic Analysis.
2. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Principles of Practical Chemistry, Sultan Chand & Sons.

S. Giri, D. N. Bajpai. and O. P. Panday, Practical Chemistry Vol. II S. Chand & Company

Programme: M.Sc. Chemistry Course Code:15PCH2CP2
Core Practical: Organic Chemistry–I
Year: I Semester: I &II Credits: 3 Total Hours: 3 x 30 = 90

A. Analysis of two component organic mixtures.

Separation and identification of compounds.

B.Green synthesis involving the following reactions using Microwave oven and Sonicator.

Acylation, halogenation, hydrolysis, reduction, oxidation, Schiff base preparation and Chalcones preparation.

C.Preparation illustrating the following reactions.

Cannizzaro reaction, Perkin reaction, Reimer – Tiemann reaction, Sandmeyer reaction, Skraup synthesis, Nitration and Acylation.

D. Preparation illustrating the following rearrangement.

Fries rearrangement

References

1. B. B. Day and M. V. Sitaram and T. R Govindachari, Laboratory Manual of Organic Chemistry. Allied Publishers Limited.
2. Gnanprakasam and Ramamurthy, Organic Chemistry Laboratory Manual, Ananda Book Depot, Chennai.
3. Jagmohan, Advanced Practical Organic Chemistry, Vol. I & II.

Programme: M.Sc. Chemistry Course Code:15PCH2CP3
Core Practical: Physical Chemistry–I
Year: I Semester: I &II Credits: 3 Total Hours: 4 x 30 = 120

Non-Electrical experiments:

1. Heat of solution from solubility.
2. Heat of solution by calorimetry.
3. Molecular weight determination by Rast method using digital Beckmann thermometer.
4. Determination of activity and activity co-efficient by freezing point method.
5. Distribution coefficient and determination of equilibrium constant.
6. Thermal analysis of simple binary systems.

Electrical experiments

7. Determination of pH and pKa values using quinhydrone and glass electrodes; Potentiometric titrations. (Acid – base, redox and precipitation).
8. Determination of solubility of sparingly soluble salt by EMF method.
9. Determination of activity coefficients from EMF data.

References

1. S.R. Palit and S.K. De, Practical Physical Chemistry Science Book Agency, Calcutta.
2. P.C. Sharma and Agarwal, Goel Publishing House, Meerut.
3. V. Venkateswaran, R. Veeraswamy and A. R. Kulaindaivelu, Practical Physical Chemistry, S. Chand & Sons.
4. J. B. Yadav, Advanced Physical Practical Chemistry, Goel Publications.

Programme: M.Sc. Chemistry Course Code: 13PCH3C07
CORE: Physical Chemistry–II*(Thermodynamics)*
Year: II Semester: III Credits: 5 Total Hours: 5 x 15 = 75

UNIT - I

Thermodynamics of non-ideal systems-concept of chemical potential, Gibbs-Duhem equation, variation of chemical potential with temperature and pressure. Concept of fugacity of gases, determination by graphical method and from equation of state. Variation of fugacity with temperature and pressure. Fugacity and standard state of non-ideal gases, fugacity coefficient. Definition of activity and activity coefficient. Variation of activity of gas with pressure and temperature. Standard states. Determination of solvent activity by vapour pressure method, cryoscopic method, activity of one component from that of other component (Gibbs-Duhem equation), mean activities of electrolytes. Determination of activity of solute.

UNIT - II.

Probability: Definition and laws of probability. Thermodynamic probability. Boltzmann expression of entropy. Probability and the third law. Statistical meaning of the third law and apparent exceptions. Irreversible or non-equilibrium thermodynamics. Phenomenological laws and Onsager's reciprocal relations, linear phenomenological relations - conjugate flows. Entropy production - examples of entropy production, Prigogine's principle of minimum entropy production, entropy production in coupled phenomena, Seebeck effect, Peltier effect.

UNIT - III.

Maxwell's distribution law of molecular velocities in an ideal gas. Experimental verification of Maxwell's distribution law. Evaluation of average velocity, root mean square velocity and most probable velocity from distribution law. Maxwell's distribution of molecular energies. The principle of equipartition of energy and the calculation of heat capacities of ideal gases. Limitations of the principle of equipartition of energy. Maxwell - Boltzmann statistics. Stirling's approximation, Langrangian multipliers. Maxwell Boltzmann distribution law. Evaluation of alpha and beta in Maxwell-Boltzmann distribution law. Limitations of Maxwell-Boltzmann distribution law.

UNIT - IV.

Partition function: Definition, justification of nomenclature. Microcanonical and canonical ensembles. Molecular partition function and Canonical partition function. The relation between the total partition function of a molecule and the separate partition function. Translational partition function. Entropy of monoatomic gases, rotational partition function. Effect of molecular symmetry on rotational partition function. Ortho and para hydrogen. Vibrational partition function. Electronic partition function, Nuclear partition function. Evaluation of thermodynamic function E, H, S, G, Cv and Cp from partition functions. Calculation of equilibrium constants of reactions involving ideal gases from partition functions

UNIT - V

Heat capacities of solids - Einstein and Debye theories of heat capacities of solids. Bose-Einstein and Fermi - Dirac statistics. Bose - Einstein distribution law. Plank distribution law for black - body radiation. (Bose - Einstein ideal photon gas) Bose - Einstein condensation. Fermi - Dirac Distribution law, ideal Fermi - Dirac gas - electron gas in metal - Fermi energy.

References:

1. L.M. Klotz and R.M. Rosenberg, Chemical thermodynamics, W.A.Benjamin (1974).
2. J.F. Lee, F.W. Sears and L. Turcotte, Statistical Thermodynamics, Addision – Welsley (1973).
3. M.C. Gupta, Statistical thermodynamics, New Age International (1990).
4. S. Glasstone, Thermodynamics for chemists, affiliated East West press (1964).
5. F.T. Wall, Chemical Thermodynamics, Freeman and Company (1965).
6. L.K. Nash Chemical Thermodynamics II, Addision Wesley Publishing (1976).
7. Gurdeep Raj Advanced Physical Chemistry, Goel Publishing House (2012).

Programme: M.Sc. Chemistry Course Code: 13PCH3C08
CORE: Organic Chemistry–III*(Chemistry of natural products)*
Year: II Semester: III Credits: 5 Total Hours: 5 x 15 = 75

UNIT - I.

Terpenoids-Isolation, classification, isoprene rule and special isoprene rule. Structural elucidation and synthesis of zingiberene, β - eudesmol, caryophyllene and abietic acid and biosynthesis of terpenoids.

UNIT - II

Cholesterol-structural elucidation (synthesis not required) - conversion of cholesterol into the testosterone and progesterone. Ergosterol-Structure - conversion into progesterone. Structural discussion of vitamin - D, testosterone and progesterone. Oestrone-Structure and Hughes *et al* synthesis -Equilenin - structure and synthesis. Biosynthesis of steroids.

UNIT- III.

General methods of ascertaining structure of alkaloids. Structural elucidation and synthesis of quinine, morphine, codeine, thebaine, reserpine and brucine. Structure of cortisones.

UNIT - IV.

Polypeptides-General principles of polypeptides synthesis, Bergmann and Sheehan *et al* methods and Solid state Peptide Synthesis. Proteins-characteristics, Classification, end group analysis, primary, secondary, tertiary and quaternary structures. Oxytocin - structure and synthesis. Enzymes and coenzymes, biosynthesis of proteins, Structures of RNA and DNA and their biological importance.

UNIT – V.

Natural Plant Pigments and co-pigments: Anthocyanins – structure of anthocyanidins and synthesis. Flavones and isoflavones – structure and synthesis. Baker – Venkataraman synthesis and Kostanecki synthesis. Flavonol – structure and synthesis.

Chemotherapy: Penicillin – structural elucidation and synthesis. Sulpha drugs – prepartion and uses of sulpha pyridine, sulphathiazole and sulphaguanidine. Mode of action of sulpha drugs.

References:

1. I. L.Finar, Organic chemistry Vol.I & II, ELBS Longmann Group.(2011).
2. O.P. Agarwal, Natural Product Chemistry, Goel Publishing House(2001).
3. Gurdeep R. Chatwal, The Chemistry of Organic Natural Products Vol. I & II , Himalaya Publishing House (2009).

Programme: M.Sc. Chemistry Course Code: 19PCH3C09
CORE–10: CORE: Computational Chemistry and Molecular Modelling
Year: II Semester: III Credits: 5 Total Hours: 5 x 15 = 75

Unit I : Molecular Mechanics

Force fields and molecular representations of matter - potential energy functions, inter- and intra-molecular interactions, empirical parameters, constraints and restraints, united atom and coarse-grained approaches, non-pairwise interactions. Energy minimization techniques- steepest descent, conjugate gradient, Newton-Raphson, simulated annealing, branch-and-bound and simplex.

Unit II : Molecular Dynamics

Elementary concepts of Ensembles and fluctuations, non-bonded cutoffs, long-range interactions, periodic boundaries, partition function, ensemble averaging and ergodicity. Trajectory analysis - conformational analysis and normal mode analysis. Brownian dynamics, free energy perturbation methods and Monte Carlo simulation.

Unit III : Quantum Mechanics

Basis set: Slater and Gaussian functions, contractions, polarization and diffuse functions, split-valence sets, correlation-consistent sets, core-valence sets, general contractions.

Semi-empirical method: π-methods, valence electron methods - extended Hückel, neglect of differential overlap methods - Austin Model 1, Parameter Model 3.

Ab initio theory: restricted and unrestricted Hartree-Fock, electron correlation, many body perturbation theory, coupled cluster theory and multi configuration self-consistent field theory.

Density functional theory: homogeneous electron gas, Coulomb hole, exchange hole, use of density functional theory in quantum chemistry, Kohn-Sham equations, exchange, correlation and hybrid functional.

QM/MM Method: Mixed methods like the combination of quantum chemical methods and molecular mechanics (QM/MM) for the description of biochemical problems with specific reference to the interaction between drug and receptor.

Unit IV : MM Modelling

MM Modelling I: Biomolecular structure modelling, visualization and database

MM Modelling II: Parameterization of force field

MM Modelling III: Ligand docking and binding pocket analysis

MM Modelling IV: Tool handling

MM Modelling V: Solvation modelling explicit *vs* implicit

MM Modelling VI: Energy minimization techniques and conformation analysis

MM Modelling VII: Molecular dynamics simulation and analysis

MM Modelling VIII: Monte Carlo simulation in chemical and biochemical applications

Unit V : QM Modelling

QM Modelling I: Electronic structure building

QM Modelling II: Basis Sets and Basis Set Superposition Error

QM Modelling III: Single point and geometry optimization calculation

QM Modelling IV: Atomic charges, dipole moment, polarizability and hyper polarizability

Electronic spin - $\hat{S}^2$ operator and degeneracy

Group theory - molecular point groups and term symbols

QM Modelling V: Vibrational frequency analysis, symmetry analysis, harmonic vs fundamental frequencies, zero-point vibrational energies, Hessian index and distinguishing minima from transition states

QM Modelling VI: Reaction profiles in gas phase reaction, solvent effects, thermodynamic properties and intrinsic reaction coordinates analysis

QM Modelling VII: Prediction of theoretical UV-vis, IR and NMR Spectroscopy

QM/MM Modelling VIII: Protein-Ligand interaction, modelling enzymatic reaction profile

References

1. F. Jensen, *Introduction to Computational Chemistry*, Wiley, New York, 1999.
2. Christopher J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, 2nd Ed. Wiley & Sons, New York, 2004.
3. Andrew R. Leach, *Molecular Modelling: Principles and Applications*, 2nd Ed., Prentice Hall, 2001.
4. David Young, *Computational Chemistry: A Practical Guide for Applying Techniques to Real World Problems*, John Wiley & Sons, 2004.
5. A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry, Introduction to Advanced Electronic Structure Theory*, 1st Ed, Dover, 1989.

Programme: M.Sc. Chemistry Course Code:13PCH3EL3
Elective:Organic Reactions and Reagents
Year: II Semester: III Credits: 4 Total Hours: 5 x 15 = 75

Unit-I

Molecular rearrangements - mechanism and applications of Wagner-Meerwein, Wolf, Sommelet-Hauser, Beckmann, Neber, Baeyer- Villiger oxidation, Dakin, Steven, Favorskii, Orton, Dienone-phenol, Benzidine, Fries and Photo Fries rearrangements.

Unit-II

Preparation and synthetic applications of organometallic compounds- Organolithium, Organozinc, Organocadmium, Organomercury, Organolead, Organoaluminium Organoboranes compounds and Grignard reagents.

Unit-III

Mechanism and applications of Named reactions- Arndt- Eistert synthesis, Elbs persulphate oxidation, Leuckart, Pechmann, Reformatsky, Wittig, Sandmeyer, Ullmann, Gomberg, Willgerdot, Wurtz, Fittig and Umpolung reactions.

Unit-IV

Reagents in organic synthesis-Preparation and applications of NBS, Osmium tetroxide, ozone, periodic acid, $Pd/BaSO_4$, Selenium, Selenium dioxide, Sodium borohydride, Lead tetra acetate, DDQ, DCC, PPA, B_2H_6 and C_6H_5COOOH.

Unit-V

Problems in organic chemistry using basic chemical reactions and elemental composition- involving hydrocarbons, aromatic hydrocarbons, alkyl halides, alcohols, aryl halides, phenols, carbonyl compounds, carboxylic acids, esters, nitro compounds, amines, nitriles. (Spectral data should not be included)

Text & Reference Books

1. O. P. Agarwal, Reactions and Reagents, Goel Publishing House (2006).
2. S. N. Sanyal, Reactions, Rearrangements and reagents, BharathiBhawan Publishers (2008).
3. V. K. Ahluwalia and R. K. Parashar, Organic Reaction Mechanisms, Narosa Publishing House (2002).
4. P. L. Soni and H. M. Chawala, Text Book of Organic Chemistry, Sultan Chand & Sons (2007).
5. Jagadamba Singh and L. D. S. Yadav, Advanced Organic Chemistry, PragatiPrakashan (2004).

Programme: M.Sc. Chemistry Course Code: 13PCH4C10
CORE: Physical Chemistry–III*(Chemical Kinetics and Electrochemistry)*
Year: II Semester: IV Credits: 4 Total Hours: 5 x 15 = 75

UNIT – I

Theories of reaction rates: Hard sphere collision theory of gas-phase reaction, potential energy surfaces, and absolute reaction rate theory – formulation in terms of partition function, relation between activated complex theory and hard sphere collision theory, thermodynamic formulation of activated complex theory (ARRT). Kinetic isotopic effects. Reactions in solution – comparison between gas-phase and solution reactions, cage effects. The influence of solvent on the reactions between ions and neutral molecules. Influence of ionic strength on rates of reactions in solution. Primary and secondary salt effects. Influence of pressure on rates of reactions in solution.

UNIT – II

Kinetic treatment of complex reactions: Parallel reactions of the same order (first and second order), reversible reactions of the same order (first), first order forward and second backward, consecutive first order reactions. Steady state approximation, chain reactions and explosions. Fast reaction – definition – study of fast reactions – flow method, pulse method, relaxation method, shock-tube method, nuclear magnetic resonance method.

UNIT – III

Homogeneouscatalysis**:** Specific and general acid-base catalysis, Bronsted catalysis law.Acidity functions – definition – significance, enzymecatalysis (single substrate reaction only), Michaels-Menten Kinetics, influence of pH and temperature on enzyme catalysis. Surface phenomenon –physisorption and chemisorption. Adsorption isotherms: Freundlich, Gibbs, Langmuir and BET. Kinetics and mechanism of heterogeneous catalysis (Langmuir – Hinshelwood and Langmuir – Rideal - Eley).

UNIT –IV

Activity, activity coefficient, ionic strength – Debye-Huckel limiting law. Dynamic electrochemical process at electrodes – electrical double layer – Helmholtz, Gouy-Chapman and Stern models. Corrosion- classification of corrosion processes, conditions for the occurrence of corrosion processes, electrochemical principles of corrosion, prevention of corrosion.

UNIT – V

Electrokinetic phenomena: Electrolytic oxidation and reduction. Voltametry and polorography – current – voltage relationships. Migration current,diffution current, residual current, half - wave potential. Ilkovic equation, dropping mercury electrode, applications of polarography. Amperometric titrations. Fundamental principles of coulometry – constant current and controlled potential methods – primary and secondary titrations.

References

1. K.J. Laidler, Chemical kinetics, Harper and Row publication (1965).

2. W.J. Moore, Physical Chemistry, Longmann's (1975).
3. S. Glasstone, An Introduction to Electrochemistry, affiliated East–West press (2004).
4. L.L. Andropov, Theoretical electrochemistry, Mir Publishers (1972).
5. Raj Narayan, An Introduction to Metallic Corrosion and its Prevention, Oxford and IBH Publishing Co(1983).
6. P.W. Atkins, Physical Chemistry VIEdition, Oxford University (1998).
7. Gurudeep Raj, Advanced Physical Chemistry, Goel Publishing House. (2012).

Programme: M.Sc. Chemistry Course Code: 17PCH4EL4
Elective:Green and NanoChemistry
Year: II Semester: IV Credits: 4 Total Hours: 5 x 15 = 75

UNIT I

Introduction to nanotechnology: Basic ideas and terminology. Classification based on dimension. Various nanostructures: Nanowires, nanorods, nanoballs, nanotubes and nanofluids. Fullerenes and graphenes (basic ideas only). Synthetic techniques of nanomaterials: Top down and bottom up approaches-lithography. Physical methods: Laser ablation, evaporation and sputtering. Chemical methods: sol-gel synthesis, co-precipitation, microwave and sonochemical methods. Synthesis and uses of certain nanoparticles: Gold, silver, zinc oxide, iron oxide and TiO_2.

UNIT –II

Characterization of nanomaterials by UV, Fluorescence, X-Ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Atomic force microscopy (AFM) and Scanning tunneling electron microscopy (STEM). Properties of nanoparticles:Optical properties, magnetic properties-diamagnetic, paramagnetic, ferromagnetic and super paramagnetic properties. Size dependent properties-coercivity and saturation magnetization. Applications of nanoparticles in the fields of medicine, energy sector, catalysis, water purification and automobiles. Nanopollution- safety and ethics.

UNIT III

Introduction of Green Chemistry-Twelve principles of green chemistry and atom economy calculations. Microwave assisted synthesis: Microwave heating, advantages of microwave exposure. Organic synthesis in water: Hofmann elimination, hydrolysis of benzyl chloride, hydrolysis of methyl benzoate. Organic synthesis in organic solvents: Esterification and synthesis of chalcone. Solvent free synthesis-Fries rearrangement. Ultrasound assisted reactions: Homogeneous reactions: Curtius rearrangement, annulations and Diels-Alder reaction. Heterogeneous reactions: Esterification, saponification and reduction.

UNIT IV

Organic synthesis in benign green solvents: Water- Pinacol coupling, Claisen rearrangement, Wittig-Horner reaction, Heck reaction and Strecker synthesis. Super critical carbon dioxide:Properties and its applications in asymmetric synthesis, polymerization, Freidel-Crafts reaction and hydrogenation.Ionic liquids: Types,

preparation and properties. Task specific ionic liquids- Bronsted acidic and basic ionic liquids. Use of ionic liquids in the synthesis of cyclic carbonates, 1-acetylnaphthalene and epoxides. Organic synthesis using phase transfer catalysts (PTC): Mechanism, types and advantages of PTC. Applications of PTC in the synthesis of Benzoin and flavones.

UNIT V

Applications of Green Chemistry for Cleaner environment:Super critical carbon dioxide in dry cleaning, as a cleaning solvent in the manufacture of ICs and computer chips. Biodegradable polymer from renewable sources - polylactic acid. Closed loop recycling of PET. Thermal polyaspartate as antiscalant. H_2O_2-eco friendly bleaching agent in paper industry. Yttrium oxide-eco-friendly corrosion inhibitor.TiO_2- as green photocatalyst for destroying hazardous pollutants.

Reference Books

1. Environmental Chemistry with Green Chemistry, Ashim. K. Das and Madhua. Das, Books and Allied Pvt. Ltd. (2012)
2. Green Chemistry A Text Book V. K. Ahluwalia, Narora Publishing House.(2013)
3. Green Chemistry-Greener Alternatives to synthetic alternatives to synthetic organic transformations,V. K. Ahluwalia, Narora Publishing House. (2011)
4. A Text Book of Nano Science and Nano Technology, T. Pradeep Tata McGraw Hill Publishing Company Ltd. (2012).
5. Nano Technology, S. Shanmugam, MJP Publishers .(2012)
6. Text Book of Nano Science and Nano Technology, R. S. Murthy, P. Shankar, Baldev Raj, B. B. Rath and James Murday, University Press (2012)
7. Introduction to Nano Science and Nano Technology, K. K. Chattopadhyay and A. N. Banerjee, PHI Learning Pvt Ltd (2012)

Programme: M.Sc. Chemistry Course Code: 17PCH4EL5
Elective: Medicinal Chemistry
Year: II Semester: IV Credits: 5 Total Hours: 5 x 15 = 75

UNIT I

Introduction to drugs: requirements of ideal drugs, sources and classification. Drug design – aim and factors governing drug design. Adsorption, Distribution, Metabolism, Excretion and Toxicity (ADMET) and Quantitative Structure Activity Relationship (QSAR). Clark and Paton's theory.

UNIT II

Anesthetics – requirements of anesthetics – classification. General anesthetics – classification and mode of action. Inhalation anesthetics - synthesis, advantages and disadvantages of ether and chloroform. Intravenous anesthetics – synthesis of thiopental sodium and ketamine hydrochloride.

Local anesthetics – requirements, classification, synthesis of benzocaine and dimethisoquin.

UNIT III

Sedatives and Hypnotics – synthesis of phenobarbitone and paraldehyde. Anticonvulsants – synthesis of phenytoin sodium and troxidone - mode of action of anticonvulsants. Gastrointestinal agents – antacids – synthesis of magnesium carbonate, aluminium hydroxide gel and magnesium trisilicate.

UNIT IV

Central nervous system (CNS) stimulants – mode of action, synthesis of caffeine and nikethamide.

Antipyretic analgesics – mode of action, synthesis and uses of paracetamol, aspirin and salol.

Expectorants and antitussives – synthesis of acetylcysteine, guaifensin and benzonatate.

Disinfectants and antiseptics – distinction and types.

UNIT V

Antibiotics – requirements of antibiotics – classification. Penicillin, chloramphenicol, tetracyclines and streptomycin - structure activity relationship.

Cardiovascular drugs – mode of action. Synthesis of diazoxide and clonidine.

Introduction to anti- HIV and anti- cancer drugs.

References

1. Ashutosh Kar, Medicinal Chemistry, New Age international Publishers, New Delhi, Edn .2
2. G.R. Chatwal, Pharmaceutical Chemistry, Organic Volume II, Himalaya Publishing House, New Delhi.
3. V. N. Rajasekaran, Pharmaceutical Chemistry-I, Theory and Practical, Sun Publications, Chennai-31.

Programme: M.Sc. Chemistry Course Code:15PCH4CP4
Core Practical:Inorganic Chemistry–II
Year: II Semester: III &IV Credits: 3 Total Hours: 3 x 30 = 90

1. Titrimetry: oxidation using ceric salts; complexometric titration involving estimation of calcium, magnesium, nickel, zinc and hardness of water using EDTA.

2. Chromatography: Column, Paper, thin layer and ion – exchange. (Demonstration)

3. Preparation of the following inorganic complexes: Pentathioureadicuprous nitrate, Potassium trioxalatoferrate(III), trans-Potassiumdiaqua(dioxalato)chromate(III), Hexaamminecobalt (III) chloride and Ammoniumhexachlorostannate(IV).

4. Quantitative estimation:
Mixture of cations involving volumetric and gravimetric estimation:
Copper and nickel, copper and zinc, copper and magnesium, iron and nickel, iron and Magnesium, and calcium and barium.

References

1. V. Venkateswaran, R. Veeraswamy and A. R. Kulandaivelu, Principles of Practical Chemistry, Sultan Chand & Sons.
2. S. Giri. D. N. Bajpai and O. P. Panday, Practical Chemistry Vol. I & II S.Chand & Company
3. J. Bassart, R. C. Dennay, G. H. Jeffery and Mendham, Vogels text book of qualitative Inorganic analysis, The ELBS & Longman.

Programme: M.Sc. Chemistry Course Code:15PCH4CP5
Core Practical: Organic Chemistry–II
Year: II Semester: III &IV Credits: 3 Total Hours: 3 x 30 = 90

1. Quantitative Estimation:

Phenol, aniline, acetone, glucose (Bertrand's and Fehling's methods) nitro, amino and methoxy group, and unsaturation.

2. Analysis of Oil (Reichart – Meisel value, Iodine value, Saponification value and acetyl value)

3. Extraction and estimation of active constituents: (Group experiment)

a) Lactose from milk
b) Caffeine from tea leaves.
c) Nicotine from Tobacco extract.
d) Citric acid or ascorbic acid from a tablet or from a natural source.

4. Preparations: At least five two-stage preparations from literature.

References

1. B.B. Day, M.V. Sitaram and T.R. Govindachari, Laboratory Manual of Organic Chemistry, Allied Publishers Limited.
2. Gnanprakasam and Ramamurthy, Organic Chemistry Laboratory Manual, Ananda Book Depot, Chennai.
3. Jagmohan, Advanced Practical Organic Chemistry Vol. I & II.

Programme: M.Sc. Chemistry Course Code:15PCH4CP6
Core Practical: Physical Chemistry–II
Year: II Semester: III &IV Credits: 4 Total Hours: 4 x 30 = 120

A. Electrical experiments:

1. Determination of
   i. Equivalent conductance of a strong electrolyte and verification of Debye – Huckel Onsagar law
   ii. Verification of Ostwald dilution law and determination of molar conductance at infinite dilution of weak electrolyte using Kohlrausch's law.
2. Conductometric determination of pKa of a weak acid.
3. Determination of the solubility of a sparingly soluble salt.
4. Conductometric titrations:
   i. Acid –Base Titration -Determination of the strength of strong acid, weak acid and mixture of acids.
   ii. Precipitation titration - Determination of the strength of KCl,KI and KCl and KI in the mixture.

B. Non-Electrical equipments

1. Determination of the strength of the acids from the ratio of rate constants, for the hydrolysis of an ester
   ii. Evaluation of Arrhenius parameters using acid hydrolysis of an ester.
   iii. Base catalysed hydrolysis of an ester
2. Rate of reaction between persulphate and iodide ions, study of salt effects over the persulphate iodide reaction.
3. Evaluation of catalytic constant of strong acids for the iodination of acetone or hydrolysis of an ester.
4. Adsorption Experiments: Adsorption of oxalic and acetic acid on activated charcoal-Freundlich – isotherm.

References

1. S. R. Palit and S. K. De, Practical Physical Chemistry Science Book Agency, Calcutta.
2. P. C. Sharma and Agarwal, Practical Physical Chemistry, Goel Publishing House, Meerut.

Course Title	:	CORE: **Project Work and Viva-Voce**	Course Code	:	13PCH4PRO
Year	:	II	Semester	:	III & IV
Hours/Week	:	5	Credit	:	5

- Identification of research problem.
- Literature Survey of the work.
- Planning and execution of experimental studies.
- Data collection and Data analysis.
- Report writing and project submission.