Indira Gandhi National Tribal University, Amarkantak (MP)

Ph. D. Course Work Syllabus of Chemistry

Core Paper	Course code	Title of the course	Credits	Marks
	PCC- 1101	Research Methodology	4	100
	PCC- 1102	Computer Applications and Data Analysis	4	100
	PCC- 1103	Research & Publication Ethics	2	50
Discipline Specific Elective Paper (Opted any one of the DET Course)				
DSET	CHE DET 1104-1115	**Discipline Specific Elective Theory (DET) paper opted from any one of the following courses**	4	100
	CHE DEP 1116	Chemistry Practical	2	50
		Total	16	400

Discipline Specific Elective Theory

Course Code	Title of Paper	Credit	Marks
CHE DET 1104	Advanced Analytical Chemistry	04	100
CHE DET 1105	Advanced Organometallic Chemistry	04	100
CHE DET 1106	Modern Physical Methods in Chemistry Research	04	100
CHE DET 1107	Advanced Materials Chemistry	04	100
CHE DET 1108	Principles of X-ray Diffraction and Electron Microscope	04	100
CHE DET 1109	Advanced Electro Chemistry	04	100
CHE DET 1110	Polymers Chemistry	04	100
CHE DET 1111	Chemistry of Natural Products	04	100
CHE DET 1112	Advanced Synthetic Organic Chemistry	04	100
CHE DET 1113	Advanced Heterocyclic Chemistry	04	100
CHE DET 1114	Bioorganic and Drug Chemistry	04	100
CHE DET 1115	Molecular Recognition & Supra Molecular Chemistry	04	100

*** Notes:**

- **Research scholars those who studied above mentioned courses in their PG Programme they must opt different course.**
- **All the elective papers will be offered as suggested by the concern DRC.**

PCC – 1101

RESEARCH METHODOLOGY

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: An Overview of Research Methodology

Research concept, steps involved, identification, selection and formulation of research problem, justification, hypothesis; literature collection- textual and digital resources (internet)

Unit – II: Research Design, Data Collection &Interpretation

Research design; sampling techniques, collection and documentation, presentation, analysis and interpretation of data

Unit – III: Scientific Writing and Formulation of Scientific Communication

Forms of scientific writing- Article, notes, reports, review article, monographs, dissertations, popular science articles, bibliographies

Outline preparation, drafting title, sub titles, tables, illustrations; Formatting tables- title, body footnotes; figures & graphs- structure, title and legends, Impact factor, citation indices, plagiarism

Unit – IV: Good Laboratory Practices and Safety Measures

Recording and storage/ retention of recorded materials, Maintenance of equipments, Storage and disposal of hazardous materials (chemical and biological), Management and user responsibilities in proper utilization of the facilities, Handling of radiation, Bio-hazardous and other toxic experimental materials

Suggested Readings:

1. Research Methodology - Methods & Techniques, CR Kothri CR (1990), VishvaPrakashan, New Delhi.
2. Research Methodology & Statistical Techniques, S Gupta (1999) Deep & Deep Publications, New Delhi.
3. Research Methodology for Biological Sciences, N Gurumani (2007), MJP Publishers, Chennai.
4. Principles and techniques of Biochemistry and Molecular Biology, 7th Ed: K. Wilson, J. Walker, Cambridge Univ. Press. UK
5. An Introduction to Practical Biochemistry, 3rd Ed : D. T. Plummer, Tata-McGraw Hill
6. Modern Experimental Biochemistry and Molecular Biology 2nd Ed: R. Boyer
7. Benjamin/Cumin
8. Physical Biochemistry, 2nd Ed: D.M. Freifelder, Freeman Press.

9. Analytical Biochemistry, 3rd Ed. D. Holme, J. Peck, Tata McGraw Hill.
10. Experimental Biochemistry, 3rd Ed: R. L. Switzer, L.F. Garrity, Freeman Press

PCC – 1102

COMPUTER APPLICATIONS AND DATA ANALYSIS

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Computers, operating systems and useful software

MS-windows and Linux; utility of Latex, MS-Office and LibreOffice for presentation and communication of research. Spreadsheets: Excel and SPSS; importing data files to statistical software; Using SPSS / R: creating variables, data entry; Descriptive data analysis: Frequencies cross tabulations and layers; Graphical tools available with Excel / R / Origin.

Unit – II: World Wide Web and Research

Electronic mail; E-Journals and E-library; using research specific search engines like Google Scholar; Journal indexing databases: SCOPUS and Web of Science; Useful research networking platforms: Academia, Linkedin and Research Gate; Showcasing research profiles at platforms like ORCID, Publons, Google Scholar, Loop and Microsoft Academic; Working with reference management tools like Endnote, Zotero, Mendeley etc; Shodhganga repository and archiving of research papers. Selecting appropriate journals for publication.

Unit – III: Analyses of experimental data (Data Analyses with Statistical Software)

Terminology in experimental designs, principles of design, completely randomized design, randomized block designs, Latin square design; Analysis of experimental data; Data analysis based on ANOVA and ANCOVA models.

Unit – IV: Analyses of sample survey data (Data Analyses with Statistical Software)

Basic principles of sample surveys, different steps in a sample survey; Techniques of random sampling: simple random sampling, stratified random sampling and systematic sampling; Purposive sampling and Quota sampling.

Suggested Readings:

1. Goon A.M., Gupta M.K. and Dasgupta B. (2002): Fundamentals of Statistics, Vol. II, 8th Edn. The World Press, Kolkata.
2. Introduction to Biostatistics, L Forthofer (1995), Academic Press, New York.
3. Biostatistical Analysis, JH Zar (2006), Prentice-Hall.
4. Research Design: Qualitative, Quantitative & Mixed Method Approaches, John W. Creswell (2009), Sage Publication, USA.
5. Experimental Design & Data Analysis for Biologists. PQ Gerry & JK Michael (2002), Cambridge University Press.
6. Choosing & Using Statistics: A Biologists Guide, D Calvin (2003), Blackwell Publisher.

PCC – 1103

RESEARCH & PUBLICATION ETHICS

(Credits- 02; Contact hours - 30h; Maximum marks - 50)

Unit – I: Philosophy & Ethics (3h)

Introduction to philosophy: definition, nature and scope, concept, branches.

Ethics: definition, moral philosophy, nature of moral judgements and reactions.

Unit – II: Scientific Conduct (5h)

Ethics with respect to science and research; intellectual honesty and research integrity; scientific misconducts – falsification, fabrication and plagiarism (FFP); redundant publications – duplicate and overlapping publications, salami slicing; selective reporting and misrepresentation of data.

Unit – III: Publication Ethics (7h)

Publication ethics – definition, introduction and importance, best practices/standard setting initiatives and guidelines – COPE, WAME; conflicts of interest; publication misconduct – definition, concept, problems that led to unethical behavior vice-versa, types; violation of publication ethics -, authorship and contributionship; Identification of publication misconducts, complaints and appeals; predatory publishers and journals.

Practices –

Open Access Publishing (4h)

Open access publications and initiatives; SHERPARoMEO online resource to check publishers copyright & self-archiving policies; software tool to identify predatory publications developed by SPPU; journal finder/journal suggestion tools viz., JANE; Elsevier Journal Finder; Springer Journal Suggester etc.

Publication Misconduct (4h)

Group discussions – subject specific ethical issues, FFp, authorship; conflicts of interest; complaints and appeals - examples from India and abroad (**2h**).

Software tools – use of plagiarism tools like Turnitin, Urkund and other open source software tools (**2h**).

Databases and Research Matrices (7h)

Databases – Indexing databases; citation databases – Web of Science, SCOPUS etc**(4h).**

Research matrices – Impact factors of journals as per Journal Citation Reports, SNIP, SJR, IPP, cite score; Matrices – h-index, g-index, i10 index, altmetrics **(3h).**

Suggested Readings:

1. Bird, A. (2006). Philosophy of Science. Routledge.
2. MacIntyre, Alasdair (1967) A Short History of Ethics. London.
3. P. Chaddah, (2018) Ethics in Competitive Research: Do not get scooped; do not get plagiarized, ISBN:978- 9387480865
4. National Academy of Sciences, National Academy of Engineering and Institute of Medicine. (2009). On Being a Scientist: A Guide to Responsible Conduct in Research: Third Edition. National Academics Press.
5. Resnik, D. B. (2011). What is ethics in research & why is it important. National Institute of Environmental Health Sciences, 1-10. Retrieved from https://www.niehs.nih.gov/research/resources/bioethics/whatis/index.cfm
6. Beall, J. (2012). Predatory publishers are corrupting open access. Nature, 489(7415), 179-17. https://doi.org/10.1038/489179a
7. Indian National Science Academy (INSA), Ethics in Science Education, Research and Governance(2019), ISBN:978-81-939482-1-7. http://www.insaindia.res.in/pdf/EthicsBook.pdf

Discipline Specific Elective Theory* (DET) (opt any one)

CHE DET 1104: Advanced Analytical Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Advanced Molecular Spectroscopy & Data Interpretation (12 Hours)

Nature of electromagnetic radiation, electromagnetic spectrum, atomic, molecular and vibrational energy levels, basic instrumentation- source of radiation, monochromator, sample cells, absorber, detector, UV-Vis detector, photomultiplier, IR detector, display and recorder, single and double beam spectrophotometer, Beer Lambert law, deviation from beers law, ultraviolet and visible spectroscopy, Fluorescence and phosphorescence spectrophotometer, Fourier transform infrared spectrometer and Raman spectrometer, instrumentation, techniques and application.

Errors and Statistics: significant figures, rounding off, accuracy and precision, determinate and indeterminate errors, standard deviation, propagation of errors, confidence limit, test of significance, rejection of a result.

Unit – II: Thermal Analysis & Atomic Spectroscopy (12 Hours)

Types of thermal method, Thermogam, thermogravimetric analysis(TGA), differential thermal analysis(DTA), differential scanning calorimetry (DSC), schematic diagram for TGA and DTA instruments and their working principle, factors affecting thermogram like geometry of sample holder, furnace atmosphere, heating rate, particle size, packing of sample, weight of sample, analysis of metals or oxide in mixture, application of TGA and DTA.

Flame emission spectrometry, atomic absorption spectroscopy- principle, instrumentation, Source in AAS – Hollow cathode lamp, electrode less discharge lamp, burners, nature and property of flame, interference in AAS, difference between AAS and FES, ICP.

Unit – III: Purification Technique (14 Hours)

Chromatography

Principles of chromatographic separation, classification of Chromatographic Techniques: adsorption, partition, ion exchange and size exclusion chromatography, theory of chromatographic separation, distribution coefficient, retention time, sorption, theory of column efficiency and resolution, separation factor, retention factor. – working principle and application of Column chromatography, ion exchange chromatography, paper chromatography, Thin layer chromatography (TLC) & HPTLC: techniques and application. - Gas Chromatography and high performance liquid chromatography: Van Deemter equation,

retention time or volume, capacity ratio, partition coefficient, theoretical plate and number, separation efficiency and resolution, instrumentation and application.

Solvent extraction

Theory, efficiency, percentage extraction, separation factor, complexing agent in solvent extraction, selection of solvent.

Ion- exchange

Principle, quality of resins, ion exchange equilibrium, ion exchange capacity process, deionization of water.

Unit – IV: Electrochemical analyses (12 Hours)

Introduction to electrochemical methods, electrochemical cells, diffusion controlled limiting current, voltage scanning polarography, shape and interpretation of polarographic wave, limiting current, current – voltage relationship during electrolysis. Electrogravimetry, voltammetry, polarography, reference electrode, working electrode, auxiliary electrode, dropping mercury electrode, Principles and applications of Voltammetry, cyclic voltammetry, polarography, anodic stripping voltammetry, amperometry, coulometry, electrogavimetry.

Unit – V: Gravimetric Analysis & Quantitative Estimation (10 Hours)

Advantage of gravimetric analysis, requirement, preparation of solution, precipitating reagent, condition for analytical precipitation, saturation and super-saturation, von Weimarn equation, co-precipitation, digestion, Ostwald ripening, aggregation and agglomeration, colloidal solution, adsorption, primary and secondary layer adsorption, peptization, impurity, inclusion and occlusion, surface adsorption, post precipitation, filtration, washing and weighing precipitate mathematical calculation on gravimetry.

Basic principle of acid base indicator, Redox titration- titration of Mohr salt against $KMnO_4$, complexometric titration- EDTA titration, Eriochrome black T indicator, complexometric titration curve, direct and back titration, masking and demasking of cations, precaution in volumetric titration, titration & Justification of Fe^{3+} and Mn^{2+} salt both in complexometry and Spectrophotometry analysis.

Reference Books:

- D. C. Harris, Quantitative Chemical Analysis, 4th Ed., W. H. Freeman, 1995
- G. D.Christian & J. E. O'Reily, Instrumental Analysis, 2nd Ed., Allyn & Balon, 1986.
- I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Gary D. Christian: *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.
- C. Daniel Harris: *Exploring Chemical Analysis*, Ed. New York, W.H. Freeman, 2001.

- S. M. Khopkar: *Basic Concepts of Analytical Chemistry*, New Age, International Publisher, 2009.
- D. A. Skoog, F. J. Holler and T. A Nieman: *Principles of Instrumental Analysis*, Thomson Asia Pvt. Ltd. Singapore.

CHE DET 1105: Advanced Organometallic Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Organometallics **(12 Hours)**

Compounds with metal carbon σ and multiple bond: Haptacity complexes of Metal-alkyl, -allyl, aryl, -carbene (Fischer and Schrock type), -carbonyl, -carbines and cyclopentadienyl complexes Synthesis, bonding, stability, reactivity and decomposition pathway, Reactions in organometallic compounds. Stucture and bonding in η^2-ethylenic and η^3-allylic compounds with typical examples, structure and bonding of $K[Pt(C_2H_4)Cl_3]$, $[(Ph_3P)_2Pt(Ph\text{-}C{\equiv}C\text{-}Ph)]$. Fluxional organometallic compounds: Fluxionality and dynamic equilibria in compounds such as η^2 olefins, η^3 allyl and dienyl complexes, techniques of study.

Reactions of organometallic complexes: substitution, oxidative addition, reductive elimination, insertion and elimination, electrophilic and nucleophilic reactions of coordinated ligands.

Unit – II: **Catalysis** **(12 Hours)**

Catalysis of organometallic compounds: Ni, Pt, Pd, Co, Zn, Cd catalyst used in various organic transformation reactions.

Nanocatalysts: Used in Different photocatalytic reaction, Oxidative addition, reduction reaction, Knoevenagel Condensation Reaction, Suzuki Coupling reaction, Unsaturation reaction etc.

Unit – III: Synthesis & Characterization **(12 Hours)**

Synthesis: Synthesis of different transition/novel metal based organometallic compounds by using various techniques like diffusion method, slow evaporation method, hydrothermal method, distillation, Microwave synthesis etc.
Characterization: The single crystal was characterized by Single X-ray crystallography, FTIR

Unit – IV: Recent Developments in Organometallics Chemistry Research **(12 Hours)**

Construction, structure and property of compounds with specific topology in Organometallic Chemistry: Capsules, boxes, containers, prisms or clusters, tubes, catenanes, rotaxanes, incorporation of metal atoms through metal-ligand coordination interactions, Various organic ligands containing carboxy, imidazole or pyridine groups, which can coordinate with metal atoms, have been used to generate the desired compounds (V, Cr, Mn, Fe, Co, Ni, Cu). Particularly, flexible ligands with central aromatic core and imidazol-1-ylmethyl pendant arms, e.g. 1,3,5-tris(imidazol-1-ylmethyl)-2,4,6-trimethylbenzene and its analogues, Interesting properties: Molecular recognition, ion inclusion and exchange of these compounds, especially of the cage-like compounds, are described.

Unit – V: Inorganic Cages and Clusters **(12 Hours)**

Polymorphism of C, P and S. Structure and bonding in higher boranes and borohydrieds-Lipscomb's topological models, Wade`s rules, carboranes and metallocenecarboranes.

Metal-metal bonding (M.O. Approach), metal-metal single and multiple bonded compounds. Low nuclearity (M_3, M_4) and high nuclearity (M_5-M_{10}) carbonyl clusters: skeletal electron counting, Wade-Mingos-Louher rule, Application of isolobal and isoelectronic relationships, Nb and Ta clusters, Mo and W clusters. Cluster compounds in catalysis.

Reference Books:

- J. E. Huheey, E. A. Keiter, R. L. Keiter, and O. K. Medhi: *Inorganic Chemistry Principle of Structure and Reactivity*, Eds: 4th Pearson, New Delhi, 2006.
- F. A Cotton, G. Wilkinson, C. A. Murillo, and M. Bochmann: *Advanced Inorganic Chemistry*, Eds: 6th, Wiley-India, New Delhi, 2010.
- D. F. Shriver and P. W. Atkins: *Inorganic Chemistry*, Oxford University Press.
- Douglas, McDaniel and Alexader: *Concepts and Models in Inorganic Chemistry*, John Wiley.
- Robert Crabtree: *The Organometallic Chemistry of the Transition Metals*, 3rd Edition, Wiley.
- Collman, Hegedus, Norton and Finke: *The Principles and Applications of Transition Metal Chemistry*, 2nd Eds, University Science Books.
- Christoph Elschenbroich: *Organometallics*, 3rd Edition,
- Wei-Yin Sun, *New Developments in Organometallics Chemistry***,** Wiley

CHE DET 1106: Modern Physical Methods in Chemistry Research

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: General Principles **(12 Hours)**

Electromagnetic radiation, interaction of electromagnetic radiation with matter, absorption, emission, transmission, reflection, refraction, dispersion, polarization, and scattering. Uncertainty relation and natural line width and natural line broadening, transition probability, result of the time dependent perturbation theory, transition moment selection rules, intensity of spectral line. Born-Oppenheimer approximation, rotational, vibrational, and electronic energy levels. Fourier Transform Spectroscopy.

Unit – II: Rotational and Vibrational Spectroscopy **(12 Hours)**

Review of Microwave, Infrared Spectroscopy, FTIR, and Raman Spectroscopy

Unit – III: Electronic Spectroscopy and Magnetic Resonance Spectroscopy **(12 Hours)**

Electronic Spectroscopy: Atomic Spectroscopy Molecular Spectroscopy and Photoelectron Spectroscopy
Magnetic Resonance Spectroscopy: Nuclear Magnetic Resonance Spectroscopy; Electron Spin Resonance Spectroscopy; Nuclear Quadrupole Resonance Spectroscopy

Unit – IV: X-ray Diffraction and Mossbauer Spectroscopy **(14 Hours)**

X-ray Diffraction: Bragg condition, miller indices, Laue method, Bragg Method, Debye-Scherrer method of X-ray structural analysis of crystals, index reflections, identification of unit cells from systematic absence in diffraction pattern. Structure of simple lattice and X-ray intensity, structure factor and its relation to intensity and electron density phase problem. Description of the procedure of an X-ray structure analysis.

***Mössbauer Spectroscopy*:** Basic principles, spectral parameters and spectrum display. Application of technique to the studies

Unit – V: Microscopy **(10 Hours)**

Electron microscopy (SEM, TEM with EDX analysis). A brief historical overview of atomic force microscopy (AFM).

Reference Books:

- C. N. Banwell and E. M. McCash: *Fundamentals of Molecular Spectroscopy*, Ed. 4th, Tata McGraw-Hill, 1994.
- B. D. Cullity: *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, 1959.
- D. B. Williams and C. B. Carter: *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, 1996.

CHE DET 1107: Advanced Materials Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Chemical Crystallography (12 Hours)

***Introduction*:** Space lattice, crystal point groups, space group (working knowledge), stereographic projections, packing in solids, crystal structures of representative systems, silicates and zeolites, cements, glasses, quasicrystals, nanostructures.

***Bonding in Solids and Crystal Energetics*:** Crystal classifications, Madelung constant and Lattice energy.

Unit – II: Characterization Techniques for Solids (12 Hours)

X-ray diffraction, electron microscopy (SEM, TEM, AFM), thermal techniques (TG, DTA, DSC), spectroscopic techniques (Mössbauer, IR, UV-VIS), and physical property measurement techniques (magnetic moments-VSM/SQUID, electrical resistivity – two / four probe methods and thermal conductivity, optical band gap, XPES, XAS.

Unit – III: Electronic and Magnetic Properties Solids (12 Hours)

Electronic Properties and Band Theory of Solids: Free electron theory of metals, Band theory of solids, Bloch theorem, Kroning-Penne model, refinement of simple band theory- *k*-space and Brillouin Zones, band structure of metals, insulators and semiconductors, intrinsic and extrinsic semiconductors, doped semiconductors, *p-n* junctions.

***Magnetic Properties Solids*:** Behaviour of substances in a magnetic field, effect of temperature: Curie and Curie-Weiss law, origin of magnetic moment, ferromagnetic, antiferromagnetic and ferromagnetic ordering, super exchange, magnetic domains, hysteresis. Introduction of superconductors, Meissner effects, basic concepts of BCH theory.

Unit – IV: Defects and Phase Transitions (12 Hours)

***Defects, Nonstoichiometry and Diffusion*:** Point defects, dislocations, extended defects, clusters and aggregates, color centers, nonstoichiometry of compounds, diffusion mechanisms, Fick's law, Kirkenall effect.

***Phase Transitions*:** Critical phenomena, variety of phase transitions (ordered-disorder, Martensite-austenite, spinoidal decompositions *etc*), liquid crystals, structure-property relations (magnetic, electrical, superconductivity, optical and thermal).

Unit – V: Preparative Techniques **(12 Hours)**

***Solid State /Ball Milling*:** Decomposition and reactivity, solid state reactions, sintering process, reaction kinetics, organic solid reactions. Powder mixing, fusion, precipitation from solution, modern need for improved synthetic routes, crystal growth and thin film techniques.

Chemical Routes: Wet-chemical (Oxidation-reduction for metal nanoparticles) methods, self assembly methods, reverse micelles route, biomimetic, sonochemical, and electrochemical approaches.

***Sol-Gel Synthesis*:** Colloids, cation hydrolysis and sol formation, gel precipitation, sol-gel process for colloids, synthesis andphysical properties of metal alkoxides, development of sol-gel process from alkoxides, derived coatings, fibers and monodispersed submicron/ nanostructured oxide powders, ormosils, sialons.

***Hydrothermal/Solvothermal Approach*:** Forced hydrolysis at elevated temperatures and pressures, hydrothermal reactions using salt solutions, metal reactants and reactions involving phase transformation.

***Gas Phase Reactions*:** Gas-phase nucleation, flame hydrolyzed powders, direct - nitridation and carbothermic reduction, non-plasma gas phase reactions, plasma reactions, electron beam evaporation.

(12 Hours)

Reference Books:

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
- A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
- C. N. R. Rao and J. Gopalkrishanan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
- R. E. Newnham, *Structure Property Relations*, Springer-Verlag, 1987

CHE DET 1108: Principles of X-ray Diffraction and Electron Microscope

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Geometry of Crystal Structure **(12 Hours)**

Form of solids, space lattice, seven crystal systems; unit cell, primitive and non-primitive cell,, Bravais lattice, lattice direction and crystal planes; Miller indices of crystal planes, separation between crystal planes, reciprocal lattice

Crystal Structure; closed packed structure- hcp and ccp, rack salt (NaCl), Wurzite and zinc blend of ZnS, diamond, CsCl, Fluoride (CaF_2) and antifluoride (Na_2O), Rutile (TiO_2) *etc*.

Unit – II: Point and Space Groups **(12 Hours)**

Symmetry operation and symmetry elements, Plane of symmetry, inversion centre, proper and improper axis of rotation, product of symmetry operation, Relation among symmetry elements and symmetry operation, thirty two point groups, representation of point groups with selected examples like 222, mm2, mmm, 32 centrosymmetric and non-centrosymmetric point groups.

Space group: Triclinic P1, monoclinic C2, monoclinic C2/m, orthorhombic $P222_1$ orthorhombic F222, Tetragonal 14_1, space group and crystal structure of perovskite ABO_3 and rutile structure of TiO_2 etc

Unit – III: X-ray Diffraction by Crystal **(12 Hours)**

Properties of X-rays, production and detection of X-ray, diffraction of X-ray by crystal, Bragg's condition, Brag's law, diffractometer and diffractometer methods (Laue, rotating-crystal, and powder methods), Scherrer formula, scattering of an electron, atom, by a unit cell, structure factor, systematic absence, intensity of powder pattern line.

Determination of crystal structure, chemical analysis by X-ray diffraction, chemical analysis by X-ray spectroscopy (EDX energy dispersive X-ray spectroscopy).

Unit – IV: Electron Microscope **(12 Hours)**

Introduction: optical microscope versus electron microscopy, brief history of electron microscope, interaction of electron and matter, elastic in-elastic scattering of electron,

Instrument: scanning electron microscope (SEM), transmission electron microscope (TEM); electron source; lenses and lenses defects, apertures and resolution, electron detection and display, pumps and sample holders, calibration of imaging system, specimen preparation for TEM

Unit – V: Transmission Electron Microscope **(12 Hours)**

Forming diffraction pattern and images; principle of image contrast, bright field and dark field imaginings, and SAED and obtaining SAED, high-resolution TEM, grain boundary, phase boundary, and other imaging techniques.

Reciprocal space; diffraction from crystals; diffraction from particles, and dislocation, indexing of diffraction patterns, Kikuchi diffraction.

References Books:

- A. R. West: *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.
- L. Smart and E. Moore, *Solid State Chemistry*, Chapman and Hall, 1992.
- A. K. Cheetham and P. Day: *Solid State Chemistry Compounds*, Clarendon Press, Oxford 1992.
- C. N. R. Rao and J. Gopalkrishanan: *New Directions in Solid State Chemistry*, Cambridge Univ. Press 1997.
- D. B. Williams and C. B. Carter: *Transmission Electron Microscopy: A Textbook for Materials Science*, Plenum Press, New York, 1996.
- B. D. Cullity: *Elements of X-ray Diffraction*, Eds: 2nd, Addison-Wesley, USA, 1959.

CHE DET 1109: Advanced Electrochemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I : Fundamentals of Advanced Electrochemistry (10 Hours)

Basic electrochemistry concepts, Ideally polarizable and non-polarizable electrodes, Reference electrodes, Working electrodes, Counter electrodes, Electrified interfaces, Electrical double layer, Adsorption phenomena at electrodes, Kinetics of electron transfer, Overpotential, Exchange current density, Butler-Volmer equation – derivation and approximations, Tafel equation, Standard electrode potential, Potentiometry, Nernst equation, Modes of mass transfer, Diffusion, Faradaic vs. Non-Faradic processes, Electrolysis, Faraday's laws.

Unit – II: Electrochemical Techniques & Instrumentation (12 Hours)

Electrochemical Techniques, Electrodeposition, Voltammetry (Cyclic Voltammetry, Linear Sweep Voltammetry), Reversible and irreversible reactions, Amperometry, Coulometry, Chronoamperometry, Chronopotentiometry, Rotating electrodes, Microelectrodes, Electrochemical Impedance spectroscopy, Spectro electrochemistry, Scanning electrochemical microscopy, Electrochemical instrumentation- simple circuits.

Unit – III: Quantum-oriented Electrochemistry (10 Hours)

The Electrochemical potential of electrons in solution and their quantal energy states, The density of states in metals; Tunneling: The idea, equations of tunneling, tunneling through adsorbed layers at electrodes; A quantum mechanical description of electron transfer: The Frank-Condon principle in electron transfer; A quantum mechanical formulation of the electrochemical current density: equation; A retrospect and prospect for quantum electrochemistry.

Unit – IV: Applications of Electrochemistry (14 Hours)

Introduction of Battery, Requirement for good battery, Factors affecting the capacity of battery, Major component of battery, Primary Battery: Dry (or) Laclanche cell, Alkaline battery; Secondary Battery: Lead Acid Storage Cell, Nickel-Cadmium (Ni-Cd) battery; Vanadium Redox Flow Battery, Lithium-ion Battery; Supercapacitors; Electrocatalysis; Electrochemical Sensors; Electrolysis; Electroplating; Corrosion and its prevention.

Unit – V : Fuel cells (14 Hours)

Introduction: History of fuel cells, operating principles of fuel cells, Fuel cell types, Fuel cell applications, Fuel cell thermodynamics, Fuel cell reaction kinetics.

Polymer Electrolyte Membrane Fuel cell components, Materials, Properties and Processes: Diffusion media, Electrocatalysts, Proton Exchange membrane.

Fundamental Electrochemical Variables: Voltage, Current and Time; Basic Fuel Cell Test Station Requirements; Current-Voltage Measurements.

Transport processes in PEM fuel cells: Ion transport in an electrolyte, Electron transport, Gas-phase mass transport, Heat generation and transport.

Application in different Sectors: Stationary, transportation, space and defense sector.

Reference Books:

- Allen J. Bard & Larry R. Faulkner: *Electrochemical Methods Fundamentals and Applications,* Eds: 2nd, Wiley-India, New Delhi, 2006.
- John O'M. Bockris & Amulya K. N. Reddy: *Modern Electrochemistry, Ionics, Vol. 1,* Eds: 2nd, Springer, New Delhi, 2006.
- John O'M. Bockris, Amulya K. N. Reddy & Maria Gamboa-Aldeco: *Modern Electrochemistry, Fundamentals of Electrodics, Vol. 2A,* Eds: 2nd, Springer, New Delhi, 2006.
- D. R. Crow: *Principles and Applications of Electrochemistry,* Eds. 4th, Blackie Academic & Professional, Madras, 1994.
- James Larminie, Andrew Dicks: *Fuel Cell Systems Explained*, Wiley, 2003.
- Frano Barbir, *PEM Fuel Cells Theory and Practice,* Academic Press July 2005.
- Subramaniam Srinivasan, *Fuel Cells: From Fundamentals to Applications,* Springer, 2006.
- Gregor Hoogers: *Fuel Cell Technology Handbook,* CRC Press, Taylor & Francis Group, USA, 2002.
- David Linden, Thomas Reddy: Handbook of Batteries, Eds 3rd, Mcgraw-hill, 2002.
- G.A. Nazri, P. Balaya, A. Manthiram, A. Yamada, and Y. Yang: *Advanced Lithium-Ion Batteries Recent trends and perspectives*, Wiley-VCH.

CHE DET 1110: Polymer Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Introduction **(12 Hours)**

Importance of polymers. Basic Concept: monomers, repeat units, degree of polymerization; linear, branched, and network polymers; classification of polymers. Polymerization: condensation, addition, radical, chain- ionic- and co-ordination-, and co-polymerization; polymerization condition and polymer reaction; polymerization in homogeneous and heterogeneous systems.

Unit – II: Polymer Characterization Techniques **(12 Hours)**

Polydispersion-average molecular weight concept; number, weight and viscosity average molecular weights. Polydiversity and molecular weight distribution. The practical significance of molecular weight. Measurement of molecular weights. End group, viscosity, light scattering, osmotic, and ultracentrifugation methods. Analysis and testing of polymers-chemical analysis of polymers. Spectroscopic methods, X-ray diffraction, microscopy studies. Thermal analysis and physical testing tensile strength, fatigue, impact, tear resistance, hardness and abrasion resistance analysis.

Unit – III: Structure and Properties **(12 Hours)**

Morphology and order in crystalline polymers – configuration of polymer chains; crystal structure of polymers; morphology of crystalline polymers; strain-induced morphology; crystallization and melting polymer structure and physical properties – crystalline melting point, T_m, melting points of homogeneous series effect of chain flexibility and other steric factors, entropy and heat of fusion. The glass transition temperature, T_g, relationship between T_m and T_g, effect of molecular weight, diluents, chemical structure, chain topology, branching and cross linking. Properties requirements for polymer utilization.

Unit – IV: Polymer Processing **(12 Hours)**

Plastic, elastomers and fibres, compounding; processing techniques- calendaring, die casting, rotational casting, film casting, injection casting, blow moulding, extraction moulding, thermoforming, foaming, reinforcing, and fibre spinning.

Unit – V: Properties of Commercial Polymers **(12 Hours)**

Polyethylene, polyvinyl chloride, polyamide, polyester, phenolic resins, epoxy resins and silicone polymers. Functional polymers – fire retarding polymers and electrically conducting polymers. Biomedical polymers – contact lens, dental polymers, artificial heart, kidney, skin, and blood cells.

Reference Books:

- Fred W. Billmeyer: *Textbook of Polymer Science*, Eds: 3rd, Wiley-India, New Delhi, 2012.
- A Ravve: *Principle of Polymer Chemistry*, Eds. 3rd, Springer Science + Business Media, New York, 2012.
- J. M. G. Cowie: *Physics and Chemistry of Polymers*, Blackie Academic and Professional.
- H. R. Alcock and F. W. Iamtee: *Contemporary Polymer Chemistry*, Prentice Hall.
- V. R. Govarikar, N. V. Viswanathan, and J. sreedhar: *Polymer Science*, Wieley-Eastern.

CHE DET 1111: Chemistry of Natural Products

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Alkaloid – I **(12 Hours)**

Occurrence and isolation, biological role of alkaloids, General properties, nomenclature and classification of alkaloids on the basis of amino acid origin and present core structure. Isolation, properties and structural elucidation of quinine, Morphine (structure, synthesis, molecular rearrangement, stereochemistry and biogenesis).

Unit – II: Alkaloid – II **(12 Hours)**

Structure and biological role of nicotine, cocaine, quinine, reserpine, vincristine, morphine, caffeine, papavarine, hyocimine. Strychnine and lysergic acid.

Unit – III: Steroid **(12 Hours)**

Introduction, nomenclature of steroids, absolute configuration of steroid. Occurrence, isolation, structute elucidation and chemical properties of Cholesterol.

Unit – IV: Terpenes **(12 Hours)**

Secondary metabolites: Definition and examples; terpenes – isoprene rule; mono terpenes: structure of geraneol, limonene, alpha-pinene and camphor; sesquiterpenes: longfolene;

diterpenes: abietic acid, taxol. Structure determination of Citral and Camphor.

Unit – V: Vitamins **(12 Hours)**

Introduction, chemical properties, structure elucidation of Vitamin A, Vitamin B, Ascorbic Acid and Vitamin D. Vitamin A and its role in vision. Biological role of Vitamin D, Ascorbic Acid, Vitamin A.

Reference Books:

- I. L. Finar: *Organic Chemistry Vol. II*, 5th Edition
- S. V. Bhat, B. A. Nagaramgagi, M. Srikumar: *Chemistry of Natural Products*, Alpa Science International Ltd, 2005 by
- O. P. Agarwal: *Chemistry of Natural Products, Vol I & Vol II*, Goel publishing House, 1989

- J. R. Hanson: *Natural Products: The Secondary Metabolites*, Wiley-Vch, 1st Ed.

CHE DET 1112: Advanced Synthetic Organic Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Metal Mediated C-C and C-X Coupling Reactions (12 Hours)

Suzuki, Heck, Stille, Sonogishira cross coupling, Buchwald-Hartwig and Negishi-Kumada coupling reactions. **C=C Formation Reactions:** Shapiro, Bamford-Stevens, McMurrey reactions, Julia Lythgoe olefination and Peterson's stereoselective olefination. Olefin metathesis by Ist and IInd generation catalysts: Reaction mechanism and application in the synthesis of heterocycles.

Unit– II: Reagents of Phosphorous, Sulfur, Silicon and Boron (12 Hours)

Phosphorous Sulfur, Silicon and Boron containing compounds-preparations and their uses in organic reactions.

Unit – III: Oxidation and Reduction (12 Hours)

***Oxidation*:** Oxidation of hydrocarbons (alkanes, aromatic hydrocarbons, alkenes), Oxidation of alcohols (Chromium reagents, Manganese reagents, Other metal and non-metal based oxidants), Oxidation of ketones (α, β-unsaturated ketones, α-hydroxy ketones, Baeyer-Villiger oxidation of ketone)

***Reduction*:** Catalytic hydrogenation, Reduction by dissolving metals, Reduction by hydride-transfer reagents (Derivatives of lithium aluminium hydride and sodiumborohydride, mixed lithium aluminium hydride-aluminium chloride reagent, DIBAL-H, $NaBH_3CN$, sodium triacetoxyborohydride, Borane and derivatives, other methods of reductions).

Unit – IV: Disconnection Approach, Umpolung Chemistry and Protection-Deprotection of Functional groups

(12 Hours)

Basic principles and terminology-Target molecule, FGI, Disconnection, Synthon, Reagent and Retro-synthetic approach. **One group C-C and C-X disconnection**: (disconnection of alcohols, alkenes, and carbonyl compounds). **Two group C-C & C-X disconnections**: 1,3 and 1,5 difunctionalised compounds, α, β, unsaturated carbonyl compounds, control in carbonyl condensation, synthesis of 3,4,5 and 6 membered rings in organic synthesis. Diels-

Alder reaction, connection in retro synthesis. Umpolung in organic synthesis. Protection and deprotection for functional groups as hydroxyl, amino, carboxylic and carbonyl.

Unit – V: Some Important Organic Reactions (12 Hours)

Selective Stereoselective Organic Reactions with Alkenes: Sharpless Asymmetric Epoxidation, Asymmetric Aziridination, Dihydroxylation, Amino-hydroxylation Reactions, Oxidative cleavages of alkenes.

Green Chemistry, Supramolecular chemistry (Crown ether, Cyclodextrin and Clalixerins) and multicomponent reactions (Ugi, Passerini, Biginelli, Hantzsch reactions).

***Chemistry of Aliphatic and Aromatic Heterocyclic Compounds*:** Epoxide, Aziridine, Azitidine, Oxetane, Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions.

References Books:

- B. F. G. Johnson: *Transition Metal Cluster*, Wiley, 1980.
- R. H. Crabtree: *The Organometallic Chemistry of the Transition Metals*, Wiley-Interscience, 2005.
- G. Wikinson, F. G. A. Stone, and E. Abel: *Comprehensive Organometallic Chemistry*, Peramon, 1980.
- I. Fleming: *Frontier Orbitals and Organic Chemical Reactions*, Wiley, 1976.
- B. B. Woodward and Hoffman: *Conservation of Orbital Symmetry*, Verlag Chemie Academic Press, 1971.
- S. Warren: *Organic Synthesis: The Disconnection Approach*, John Wiley & Sons (Asia) Pte. Ltd., 2007
- W. Carruthers and I. Coldham: *Modern Methods of Organic Synthesis*, Fourth Ed. Cambridge University Press.
- T. L. Gilchrist: *Heterocyclic Chemistry*, Pearson Education, 3rd Ed.2007

CHE DET 1113: Advanced Heterocyclic Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Introduction (12 Hours)

Definition of heteroatom, Aromatic and non-aromatic heterocyclic compounds, Classification and nomenclature of heterocyclic compounds, important reactions with heterocyclic compounds i.e. oxidation, reduction and tertiary effect of Nitrogen in heterocyclic compound.

Unit – II: Non-Aromatic Heterocycles (12 Hours)

Different types of strains, interactions and conformational aspects of non-aromatic heterocycles. Synthesis, reactivity and importance of the following ring systems: Aziridines, Oxiranes, Thiiranes, Oxaziridines, Azetidines, Oxetanes and Thietanes.

Unit – III: Five and Six Membered Heterocyclics with One Hetero Atom (12 Hours)

Pyrrole, Furan, Thiophene, Pyridine, Indole, Quinoline, Isoquinoline - Synthesis and reactions [Advanced level Synthetic preparation or method applied].

Unit – IV: Five and Six Membered Heterocyclics with Two Hetero Atoms (12 Hours)

Synthesis, reactivity, aromatic character and importance of the following heterocycles: Pyrazole, Imidazole, Oxazole, Thiazole, Isoxazole, Isothiazole, Pyridazine, Pyrimidine. Pyrazine, Oxazine, thiazine, benzimidazole, benzoxazole and benzthiazole.

Unit – V: Larger Ring and Other Heterocycles (12 Hours)

Synthesis, structure, stability and reactivity of Azepines, Oxepines and Thiepines. Synthesis of Benzoazepines, Benzooxepines, Benzothiepines, Azocines and Azonines.

Reference Books:

- T. Gilchrist: *Heterocyclic Chemistry*
- R. M. Acheson: *An Introduction to the Chemistry of Heterocyclic Compounds*
- J. A. Joule & K. Mills: *Heterocyclic Chemistry*
- A. Paquette: *Principles of Modern Heterocyclic Chemistry*

- J, A. Joule & Smith: *Heterocyclic Chemistry*
- A .R. Katritzky: *Handbook of Heterocyclic Chemistry*

CHE DET 1114: Bioorganic and Drug Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Overview of Bioorganic Chemistry (12 Hours)

***Introduction*:** Definition of bioorganic chemistry, Border line of bioorganic chemistry and inter disciplinary area between chemical and biology, Weak interaction in organic and biological world, Molecular Recognition.

***Chemistry of the Living Cell*:** The structure of prokaryotic and Eukaryotic cells, Composition of living cells:

Unit – II: Carbohydrates, Proteins, Lipids, and Nucleic Acids (16 Hours)

***Carbohydrates*:** Introduction, Reactions of Monosaccharides, Interconversions, Ring structure of aldoses and ketoses, Confirmation of Monosaccharides, Disaccharides: Structure, synthesis and properties.

***Proteins*:** General structure & classification of amino acids, Abbreviation of amino acids, Essential and non essential amino acids, Synthesis of amino acids, Isoelectric point, Acid and base properties of amino acids. Protein: Naturally occurring peptides, Modern methods of peptide synthesis with protection and deprotection, Determination of sequences and basic units of a poly peptides or proteins, C- & N-terminus detection by chemical methods, Primary, secondary, tertiary and quaternary structures of proteins, Enzyme active sites, allosteric sites, and mechanism of their actions e.g. chymotrypsin, carboxypeptidase, lipases etc.

***Lipids*:** Lipid structure- acylglycerols, phosphoglycerides and sphingolipids, Biological importance of fatty acids and lipids, Bio- and chemical Synthesis of lipids.

***Nucleic Acids*:** Definition, structure and properties, base pairing, double helices, Genetic information storage, transmission and gene expression, Nucleotides and Nucleosides: Similarities and differentiation, Structure of DNA & RNA. Types of mRNA, tRNA and rRNA, Replication, transcription and translation, Genetic code, Protein biosynthesis.

Unit – III: Analogy Between Biochemical and Organic reactions (10 Hours)

Introduction to metabolism (catabolism, anabolism). ATP: The universal currency of cellular energy, ATP hydrolysis and free energy change. Agents for transfer of electrons in biological redox systems: NAD^+, FAD. Conversion of food to energy: Outline of catabolic pathways of carbohydrate- glycolysis, fermentation, Krebs cycle. Overview of catabolic pathways of fat

and protein. Interrelationship in the metabolic pathways of protein, fat and carbohydrate. Caloric value of food, standard caloric content of food types.

Unit – IV: Overview of Drug Chemistry and Basics of Drug Action (12 Hours)

Definition, classification and nomenclature of drugs, Preliminary idea of drug action: Interaction (Weak interaction in drug molecules, Chirality and drug action), Receptorology (Drug-receptor interactions, Enzyme kinetics in drug action, Enzyme inhibitors (Drug action through enzyme inhibition), Nucleic acids as targets for drug actions, NA-Alkylation, NA-strand breaking and their importance in drug action, Drug metabolism, drug deactivation and elimination.

Unit – V: Pharmaceutical Compounds: Structure and Importance (10 Hours)

Classification, structure and therapeutic uses of antipyretics: Paracetamol (with synthesis), Analgesics: Ibuprofen (with synthesis), Antimalarials: Chloroquine (with synthesis). An elementary treatment of Antibiotics and detailed study of chloramphenicol, Medicinal values of curcumin (haldi), azadirachtin (neem), vitamin C and antacid (ranitidine).

Reference Books:

- L. Stryer: *Biochemistry*, 4th Edition W. H. Freeman and Co. 1995.
- S. Zubay: *Biochemistry*, Addison-Wesely 1983.
- J. Mann; R.S. Davidson: *Natural Products: Chemistry and Biological Significance*
- H. Dugas: *Bioorganic Chemistry Frontiers Vol. 2*, ed. Springer-Verlag, 1990.
- E. E. Tamlen: *Bioorganic Chemistry*, Academic Press, 1977.
- M. Bodansky: *Peptide Chemistry: A Practical Textbook*, Springer-Verlag 1988.
- *Bioorganic Chemistry: A chemical approch to enzyme action*, Springer-Verlag 1989.
- W. Saenger: *Principles of Nucleic acid structures*, Springer-Verlag 1984.
- G. R. Chatwal: *Medicinal Chemistry*
- A. Kar: *Medicinal Chemistry*, Wiley, 2000.
- D. Lednicer: *Strategies for Organic Drug Synthesis and Design*, John Wiley 1998.
- G. R. Chatwal: *Synthetic Drugs*, Himalaya, New Delhi 1995.
- S. Hanessian, *Total synthesis of Natural product: The chiral approach Vol.III* Pergamon Press 1983.
- W. D. Foye, T. L. Lemke, and D. A. Williams: *Principles of Medicinal Chemistry (*4th Edition)
- R. B. Siwerman: *Organic Chemistry of Drug Action and Design* (Academic press, 1993).

CHE DET 1115: Molecular recognition and Supramolecular Chemistry

(Credits- 04; Contact hour- 60h; Maximum marks – 100)

Unit – I: Principal of molecular recognition (10 Hours)

Concept of molecular recognition and Supramolecular Chemistry. Host-Guest Chemistry, and its classification. Receptor, Coordination and the lock and key analogy. Thermodynamic and Kinetic Selectivity. Nature of supramolecular interactions.

Unit – II: Supramolecular Chemistry of Life (10 Hours)

Alkali metal ions in biochemistry. Porphyrins and Tetrapyrrole macrocycles. Plant Photosynthesis. Uptake and transport of oxygen in Haemoglobin. Coenzyme B_{12}.Neurotransmitter and Hormones. DNA. Biochemical self assembly.

Unit – III: Cation & Anion Binding Host (20 Hours)

Crown ether, Lariat ether and podands, Cryptands, Calix[n]arenes; Spherands; Selectivity of cation complexation; Macrocyclic, Macrobicyclic and Template effect.

Concept of Anion binding host design. Guanidium-based receptors; Organometalic receptors; Neutral receptors, Hydride sponge; Anticrown; Biological anion receptors.

Unit – IV: Binding of Neutral molecules (10 Hours)

Binding by cavitands, cyclodextrines, Molecular cleft and tweezers, cyclophanes, cryptophanes Host.

Unit – V: Supramolecular reactivity and Catalysis (10 Hours)

Catalysis by cation, anion and neutral receptors; Supramolecular metallocatalysis; Cocatalysis; Biomolecular and abiotic catalysis.

Reference Books:

1. J. W. Steed and J. L. Atwood: *Supramolecular Chemistry*, John Wiley and Sons, Ltd.
2. Jean –Marie Lehn: *Supramolecular Chemistry-Concepts and Perspectives*, VCH.
3. Hans-Jorg Schnider and Anatoly K. Yatsimirsky: *Principles and Methods in Supramolecular Chemistry*, John Wiley and Sons, Ltd.
4. Antonio Bianchi, Kristin Bowman James and Enrique Garcia-Espana: *Supramolecular Chemistry of anions*, Wiley-VCH.

CHE DEP 1116: Chemistry Practical

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

Advanced Analytical Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

Group-A: Analysis of Complex Materials

Quantitative analysis of complex materials, such as, ores and minerals, metals and alloys, industrial materials by conventional and or instrumental methods as applicable.

Model Samples

Ores, Minerals , Concentrates: Dolomite ($CaCO_3$, Mg CO_3, Fe_2O_3, SiO_2); Pyrolusite (MnO_2, MnO, Fe_2O_3); Chalcopyrite (CuS, FeS); Bauxite (Al_2O_3, Fe_2O_3, TiO_2, SiO_2); Chromite (Cr_2O_3, Fe_2O_3, MnO, SiO_2); Basic slag (Al_2O_3, Fe_2O_3, P_2O_5, SiO_2).

Metals and Alloys: Brass (Cu, Zn); Soldier / Type metal (Pb, Sb, Sn); Bronze(Cu, Zn, Sn), Aluminium bronze(Cu, Al, Fe, Mn), Steel (Cr, Mn, Ni, P).

Mixture: Chromium (III) and Mn(II) in a mixture, Iron (III) and Cu(II) in a mixture, Iron(III) and Al(III) in a mixture

At least one ore/ mineral/concentrate and one alloy should be analyzed during the laboratory session.

Group-B: FT-IR and UV assignment of synthesized metal complexes

Group-C: Presentation / Seminar

Group-D: Literature Review report

Reference Books:

- I. Vogel: *A Test book of Quantitative Inorganic Analysis* (Rev. by G.H. Jeffery and others) 5th Ed. The English Language Book Society of Longman .
- Hobert H. Willard et al: *Instrumental Methods of Analysis*, 7th Ed. Wardsworth Publishing Company, Belmont, California, USA, 1988.
- Gary D. Christian: *Analytical Chemistry*, 6th Ed. John Wiley & Sons, New York, 2004.

Advanced Organometallic Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

A. Preparation of selected inorganic compound and their studies by I.R., electronic spectra, Mössbauer and magnetic susceptibility measurements. Handling of air and moisture sensitive compounds

1. Mn_{12} Acetate Single Molecule Magnets
2. $K_2[Fe(C_2O_4)_3]$ .3 H_2O
3. $[Fe_3(\mu_3\text{-}O)(\mu\text{-}O_2CR)_6L_3]$ (L = H_2O, R= alkyl/aryl/)
4. $[Fe_3O(PhCO_2)_6(MeOH)_3](NO_3)(MeOH)_2$
5. $[Fe_8O_3(O_2CCMe_3)_6(N_3)_3(tea)(teaH)_3]\cdot 0.5(EtOH)$
6. $Cu_2(C_6H_5COO)_4(C_6H_5COOH)_2$
7. Tris(ethylenediamine)nickel(II) thiosulphate

B. Determination of crystal Structure by ORTAP file.

C. Presentation / Seminar

D. Literature Review report

References Books:

- Liz, T. *Acta Crystallogr.* ***1980***, *B36*, 2042
- Sessoli, R.; Tsai, H.-L.; Schake, A. R.; Wang, S.; Vincent, J. B.; Folting, K.; Gatteschi, D.; Christou, G.; Hendrickson, D. N. J. Am. Chem. Soc. 1993, 115, 1804.
- J-X. Daia, F-H. Wua, A. Rothenbergerb, Q-F. Zhang, *Z. Naturforsch.*, 2007, 62b, 1117 – 1122.
- M. K. Zart, D. Powell, A. S. Borovik, *Inorganica Chimica Acta*. 2007, 360(7), 2397–2402.
- V. Psycharis, C. P. Raptopoulou, A. K. Boudalis, Y. Sanakis, M. Fardis, G. Diamantopoulos, G. Papavassiliou, *Eur. J. Inorg. Chem.*, 2006, 3710–3723.
- M. Narshim, A. Saritha, B. Raju, K. A. Hussain, IJIRSET, 4(8), 2015, 7548-7555.

- Olga Botezat, Jan van Leusen, Victor Ch. Kravtsov, Arkady Ellern, Paul Kögerler and Svetlana G. Baca, Dalton Trans., 2015, 44, 20753.
- S. Pathak, N. Biswas, B. Jana, T. K. Ghorai, Advanced Materials proceeding, 2017

Modern Physical Methods in Chemistry Research/Advanced Materials Chemistry/Principles of X-ray Diffraction and Electron Microscopy/Advanced Electrochemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

1. Synthesis: A) Solid State method, (Fe_2O_3/TiO_2, Fe_2O_3/ZnO, Fe_2O_3/ZrO_2)
   B) Co-precipitation (transition metal doped ZnO, ZrO_2)
   C) Green Technique: Ag Nanoparticles, Cu NPs, Zn NPs etc.
   D) Sol-gel: ZnO, ZrO_2
   E) Synthesis of Graphene oxide nano powder
   F) Synthesis of Carbon nano tube
   G) Synthesis of nanoparticles using electrochemical methods
2. Characterization: UV, FTIR, XRD, Electron Microscopy (available of Department)
3. Application Study: Optical, Magnetic, Catalytic etc.
4. Presentation / Seminar
5. Literature Review report

Reference Books:

- Pradeep, T. *A Textbook of Nanoscience and Nanotechnology*, McGraw Hill Edu. New Delhi, (2015).
- G. L. Hornyak, J. J. Moore, H. F. Tibbals, and J. Dutta: *Fundamentals of Nanotechnology*, CRC Press, 2009

Polymer Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

1. Polymer Synthesis:

i) Free radical solution polymerization of styrene (St) / Methyl Methacrylate (MMA) / Methyl Acrylate (MA) / Acrylic acid (AA).

Purification of monomer

Polymerization using benzoyl peroxide (BPO) / 2,2'-azo-bis-isobutylonitrile (AIBN)

ii) Preparation of nylon 66/6

iii) Redox polymerization of acrylamide

iv) Precipitation polymerization of acrylonitrile

v) Preparation of urea-formaldehyde resin

vi) Preparations of novalac resin/resold resin.

2. Polymer characterization

i) Determination of molecular weight by viscometry:

Polyacrylamide-aq.$NaNO_2$ solution

ii) Determination of the viscosity-average molecular weight of poly(vinyl alcohol) (PVOH) and the fraction of "head-to-head" monomer linkages in the polymer.

iii) Determination of molecular weight by end group analysis: Polyethylene glycol (PEG) (OH group).

3. **Polymer analysis**

i) Estimation of the amount of HCHO in the given solution by sodium sulphite method

ii) Instrumental Techniques

iii) IR studies of polymers

iv) DSC analysis of polymers

v) Preparation of polyacrylamide and its electrophoresis

4. **Presentation / Seminar**

5. **Literature Review report**

Reference Books:

- Malcohm P. Stevens, Polymer Chemistry: An Introduction, 3rd Ed.
- Harry R. Allcock, Frederick W. Lampe and James E. Mark, Contemporary Polymer Chemistry, 3rd ed. Prentice-Hall (2003)
- Fred W. Billmeyer, Textbook of Polymer Science, 3rd ed. Wiley-Interscience (1984)
- Joel R. Fried, Polymer Science and Technology, 2nd ed. Prentice-Hall (2003)
- Petr Munk and Tejraj M. Aminabhavi, Introduction to Macromolecular Science, 2nd ed. John Wiley & Sons (2002)
- L. H. Sperling, Introduction to Physical Polymer Science, 4th ed. John Wiley & Sons (2005)
- Malcolm P. Stevens, Polymer Chemistry: An Introduction, 3rd ed. Oxford University Press (2005)
- Seymour/ Carraher's Polymer Chemistry, 9th ed. by Charles E. Carraher, Jr. (2013).

Chemistry of Natural Products/Advanced Synthetic Organic Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

A. Extraction

1. Extraction of caffeine from tea leaves.
2. Lycopene extraction form Tomatoes
3. Extraction of DNA from onion/cauliflower
4. Separation of amino acids by paper chromatography
5. Study of titration curve of glycine
6. To determine the saponification value of an oil/fat.
7. To determine the iodine value of an oil/fat
8. Practical Synthesis of of any one indole alkaloids.
9. If possible, extraction of any alkaloids from plants.

B. **Synthesis of Organic Compounds**:

1. Pd-catalyzed Heck reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

1. Pd-catalyzed Suzuki coupling reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

2. Pd-catalyzed Sonogishira coupling reaction (Reaction design, starting material preparation if not commercially available, reaction set-up, monitoring the reaction progress, purification and spectroscopic analysis should be carried out by each student).

3. Wittig reaction and Wittig Horner method for alkene synthesis (Any one suitable example from each reaction).

4. Oxidation and Reduction (choose any one suitable example from each category)
   (i) Oxidation of secondary alcohol to ketone
   (ii) Oxidation of primary alcohol to aldehyde
   (iii) Reduction of aldehydes by $NaBH_4$
   (iv) Reduction of ketones by $LiAlH_4$

5. Synthesis of an Imidazolidinone Organocatalyst and its application in a DA Reaction: Multistep Synthesis
   (i) Catalyst synthesis
   (ii) Diels-Alder reaction.
   (iii) Purification step
   (iv) Spectral data analysis (1H-NMR and 13C-NMR)

6. Multi component reaction: Biginelli reaction

Advanced Heterocyclic Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

1. Three member Heterocycles:

i) Epoxide synthesis from alkenes

ii) Epoxide synthesis from Halohydrin substrates

iii) Aziridination of alkenes

iv) Aziridine synthesis from amino acids

2. Five member Heterocycles:

i) Hantzsch synthesis of Pyrrole.

ii) Multicomponent reaction for synthesis of Pyrrole (Jana method).

iii) Meyer's Oxazoline synthesis from amino alcohol.

3. Fused five- or six member heterocycles:

i) Indole synthesis

ii) Quinoline synthesis

iii) Synthesis of 1-Phenyl-1,2,3,4-tetrahydroisoquinolines.

4. Basic reactions with heterocycles:

a) Treatment of Br_2 in MeOH and followed by oxidation with Amberlyst-15.

b) [3+2]-cycloaddition reaction of aziridine and carbonyl compounds in the presence of Lewid acid.

References of Books:

- *Practical Organic Chemistry* by A. I. Vogel.
- *Practical Organic Chemistry* by F. G. Mann and B. C. Saunders.

- The Organic Chemistry Journals: plz search Supporting informations of Journal of Organic chemistry, Organic Letters and Journal of American chemical Society from ACS Publication and Angew. Chem. Int. Ed. (Willey publishers); Chemical Communication (Royal Chemical Society) for appropriate experimental methods.
- *Journal of Chemical Education* **1985**, *62*, 262.

Bioorganic and Drug Chemistry/Molecular Recognition and Supramolecular Chemistry Lab

(Credits- 02; Contact hour- 60h; Maximum marks – 50)

(a) Synthesis of Following Drug Molecules:

1. Paracetamol
2. Acetanilide
3. Aspirin
4. Phenazone
5. Ibuprofen

(b) Synthesis of short peptide containing 2-3 different amino acids.

(c) Crararacterization:

1. Practices for recording the UV-visible spectra of suitable chromophoric molecules.

2. Sample preparation and recording the IR Spectra for IR-active compounds.

3. Analyze the first-order/ second order ^{1}H-NMR Spectra of any standard organic molecules (Identification of chemical shifts for all protons, measurement of coupling constant, diastereoisomers ratio, determination of chemical yields by using a standard)

4. Analyze the 2D-^{13}C-NMR spectra of any organic molecules.

5. Analytical separation of diastereoisomers and enantioisomers by using HPLC techniques and determining the enantiomeric purity (ee/er) and diastereoisomers ratio (d.r.) by HPLC chromatogram.

After completion of above hands on experiences, a student would be enabling to analyze any unknown spectroscopic datas (e.g.; UV-Visible spectra, IR Spectra, 1H-NMR spectra and 13C-NMR Spectra).

References of Books:

- Khosla, B. D.; Garg, V. C. & Gulati, A., *Senior Practical Physical Chemistry*, R. Chand & Co.: New Delhi (2011).
- Garland, C. W.; Nibler, J. W. & Shoemaker, D. P. *Experiments in Physical Chemistry 8th Ed.;* McGraw-Hill: New York (2003).
- Halpern, A. M. & McBane, G. C. *Experimental Physical Chemistry 3rd Ed.;* W.H.

Freeman & Co.: New York (2003).
- Bessler and Silverstein, Spectroscopy of Organic Compounds, JOHN WILEY, 2001.
- D. C. Pavia, G. M. Lampman, G. S. Kriz, Introduction to Spectroscopy, *3rd Edition,* THOMSON, 2007.
- Organic Spectroscopy III Edition–by William Kemp
- *Practical Organic Chemistry* by A. I. Vogel.
- *Practical Organic Chemistry* by F. G. Mann and B. C. Saunders.
- For Pd-catalyzed cross coupling reaction, recommend ACS journal's Supporting Information
- *J. Chem. Edu.* (DOI: 10.1021/acs.jchemed.5b00812)
- *Advanced Practical Organic Chemistry* by J. Leonard, B. Lygo and G. Proctor.