IA 601: Symmetry and Chemical Bonding

Learning Objectives

The learning objectives of this course are to

- (i) Illustrate the symmetry elements and symmetry operations generated by each symmetry element for a given molecule.
- (ii) Discuss the various categories of point groups and how to set up multiplication table for point groups.
- (iii) Show how to build up the character table.
- (iv) Demonstrate the scope of the symmetry and group theory to inorganic compounds.
- (v) Impart knowledge on molecular symmetry to predict molecular properties and provide hints about how the molecules change their symmetry when they take part in chemical reactions.

Course Content

- 1. **Rules of Symmetry:** Symmetry elements and operations, illustrations from Re₂Cl₄²⁻ ion, general rules for multiplications of symmetry operations, practical scheme for classification of symmetry groups, S groups, groups of very high symmetry, T_d, O_h and I_h, molecular symmetry and optical activity, molecular vibrations, dipole moment and electronic spectra.
- 2. Molecular Symmetry: Complexes of coordination number 2-8 and higher, polyhedral case and cluster complexes, fluxional compounds and their NMR spectrum.
- **3.** Mathematical Groups: Characterizing the properties of a mathematical group, multiplication table for groups of order 1-6, cyclic groups, sub groups, classes, matrix multiplication.
- 4. **Representation of Groups:** Matrices and vectors, conjugate matrices, matrix notation for geometric transformations, vectors and their scalar products, representation of groups, the great orthogonal theorem and its consequences, five important rules, character tables, representation of cyclic groups.

Learning Outcome

Upon completion of this course, the students will be able to

- (i) Identify symmetry elements and recognize symmetry operations for a molecule and state the point group a molecule belongs to.
- (ii) Acquire knowledge how to build up the character table.
- (iii) Deduce which modes of vibrations is IR/Raman active.
- (iv) Classify the atomic and molecular orbitals according to symmetry.
- (v) Ascertain the polarity and chirality of a molecule using symmetry criteria.

- 1. Chemical Applications of Group Theory, F. A. Cotton.
- 2. Molecular Symmetry and Group Theory, R. L. Carter.
- 3. Advanced Inorganic Chemistry, F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann.
- 4. Inorganic Chemistry, G. L. Miessler and D. A. Tarr.
- 5. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford.

IA 602 Coordination Chemistry

(Half Unit)

Learning Objectives

The learning objectives of this course are to

- (i) Discuss about the concepts of hard and soft acids and bases and their applications.
- (ii) Impart knowledge on stepwise and overall stability of metal ligand complexes, and how does EAN explain the stability of complex compound.
- (iii) Convey knowledge on bonding of organometallic pi-complexes like metal carbonyls and metallocenes.
- (iv) Describe ligand field theory of octahedral, square planar and tetrahedral complexes, the determining factors for 10 Dq, and photoelectron spectroscopy of complexes.
- (v) Explain the Jahn-Teller effectin octahedral transition-metal complexes.

Course Content

- 1. Complex Formation and Stability: Hard and Soft acids and bases(HSAB), concept in complex formation, magnetic properties and structure of complexes, stepwise dissociation of ML, and the overall equilibrium and stability constants, topology of complexes, stereoand constitutional isomerism, stability and EAN, chelation and stability.
- 2. Organometallic π -Complexes: Metal carbonyls, Zeise's salt, sandwich structure, ligand MOs and the matching metal atomic orbitals in metallocenes, MO diagram of Fe(C₅H₅)₂, Walsh correlation diagram and the modes of diatomic ligands, metal-metal bonds in Re₂Cl₈²⁻
- **3.** Ligand Field Splitting in Complexes: Ligand field theory of octahedral, square planar and tetrahedral complexes, factors responsible for 10Dq, photoelectron spectroscopy of complexes, photo absorption and charge transfer absorption bands.
- 4. Shapes of Complexes: Jahn Teller theorem, angular overlap model or AOM, application of AOM to octahedral, tetrahedral and square planar complexes, equivalency of d_z^2 and d_x^2 . y^2 in octahedral complexes, determining overlap integral for d-orbitals in tetrahedral symmetry.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Explain the use of terms Hard and Soft in relation to metal ions and ligands and discuss the stability of complexes in terms of hard and soft interactions.
- (ii) Understand the stability of metal complexes and recognize the types of isomers in coordination compounds.
- (iii) Understand the bonding and structure of organometallic π -compounds.
- (iv) Applyligand field theory in octahedral, square planar and tetrahedral complexes.
- (v) Realize the distortion of d⁴ and d⁹ transition metal octahedral complexes based on Jahn-Teller theorem.

- 1. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford.
- 2. Inorganic Chemistry, G. L. Miessler and D. A. Tarr.
- 3. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson.
- 4. Chemistry of the Elements, Greenwood and Earnshaw.
- 5. Chemical Structure and Bonding, R. L. Dekock and H. B. Gray.
- 6. Infrared and Raman Spectra of Inorganic and Coordination Compounds, K. Nakamoto.
- 7. Chemical Applications of Group Theory, F. A. Cotton.

IA 603: Nuclear and Radiochemistry

(Half Unit)

Learning Objectives

The learning objectives of this course are to

- (i) Impart advance knowledge on the different areas of nuclear chemistry including nuclear structure based on nuclear models, nuclear reactions and nuclear spectroscopy.
- (ii) Promote knowledge on nuclear technology, transuranium elements and hot atom chemistry.
- (iii) Describe how the electricity generated in a nuclear power plant.
- (iv) Discuss the health effects of radiation.
- (v) Inform the cosmic origin of the chemical elements.

Course Content

- 1. Nuclear Structure: Nuclear binding energy, nuclear spin and moments, nuclear potential, models for nuclear structure and properties; optical model, Fermi-Dirac model, many particle shell model, collective model, comparisons of nuclear models, nuclear parity and symmetry.
- 2. Nuclear Energy: Basic principles of chain-reacting system, reactors and their uses, reactorassociated problems, controlled thermonuclear reactions, generation of electrical energy from nuclear power stations, thermal and fast fission power reactors, fusion reactor technology.
- 3. Nuclear Spectroscopy and Instrumentation: α -, β -, γ -decay schemes, α -, β and γ -spectrometry, α -spectrometry with silicon barrier detector, high resolution γ -spectrometry with GE detectors, detection of neutrons with BF₃ detectors, Mossbauer spectroscopy and its applications.
- 4. Transuranium Elements: General ideas about transuranium elements (Z = 93-106) and their nuclear properties, their production, separation and purification, their chemistry and uses, synthesis of superheavy elements.
- 5. Hot Atom Chemistry: Formation of recoil atoms, mechanism of reactions of recoil atoms, hot atom reactions in solids, reactions of recoil tritium and carbon atoms.
- **6.** Nuclear Technology: Radiation induced chemical polymerization, surface curing of matters using γ-and UV-radiation, diagnostic and therapeutic uses of radioisotopes, ⁹⁹Tc, ¹²⁵I, ¹³¹I, ⁶⁸Ga, ⁶⁰Co, etc., γ-radiation for bone scanning, positron imaging, radiolysis of water, food preservation.
- 7. Nuclear Safety Issues: Nature of environmental radioactivity and its transfer to the human body, biomolecular effects of different types of radiation, radiation sensitivity of different organs and organisms, somatic effects of large doses on man, radiation protection standards and protective measures, radioactive wastes, recent methods to dispose critically dangerous radioactive wastes.
- 8. The Origin of the Chemical Elements: Cosmology, cosmic abundance curves, stellar evolution, steller formation, star populations, evolution of a star, stellernucleosynthesis, hydrogen fusion, helium burning : red giants, heavier elements burning, formation of elements heavier than helium, the s-, r- and p-processes, formation of the heaviest elements and supernova explosions.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Understand the nuclear structure come up by scientists with lots of different models, and principles of different detectors based on α -, β -, γ -spectrometry.
- (ii) Elucidate the production, separation, purification and uses of transuranium elements.

- (iii) Understand the mechanism of reactions of recoil atoms and interpret the diagnostic and therapeutic uses of radioisotopes.
- (iv) Explain how radiation interacts with human tissues, what the possible consequences and the remedies are, and how to store and dispose of nuclear wastes.
- (v) Understand the fundamentals of the cosmic origin of the chemical elements and the nuclear history of the universe.

Books Recommended

- 1. Radiochemistry and Nuclear Methods of Analysis, W. D. Ehmann and D. E. Vance.
- 2. Nuclear and Radiochemistry, G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller.
- 3. Introduction to Nuclear Physics and Chemistry, B. G. Harvey.
- 4. Essentials of Nuclear Chemistry, H. J. Arnikar.
- 5. Nuclear Chemistry and Its Applications, G. R. Choppinand J. Rydberg.

IA 604 Analytical Chemistry (Half unit)

Learning Objectives

The learning objectives of this course are to

- (i) Discuss about the application of statistical methods for the evaluation of laboratory data.
- (ii) Provide fundamentals of chemical analysis, including an understanding of some of the most important analytical techniques used today (titrimetric analysis, spectroscopic methods including UV-visible, and atomic absorption, electroanalysis, thermal analysis and chromatography).

(iii)

Course Content

- 1. Statistical Treatment of Data: Population and sample mean, standard deviation, relative standard deviation, coefficient of variation, variance, confidence limit, statistical tests, coefficients of correlation, regression lines, least square method.
- **2.** Complexometric Methods of Analysis: Complexation of metal ions, complexation equilibria, influence of [H⁺] on complexation, metal chelate stability, titration with chelating agent such as EDTA, NTA etc., metallochromic indicators, masking and demasking, uses of EDTA titrations.
- **3.** Solvent Extraction in Analytical Chemistry: Separation processes, liquid-liquid extraction, distribution of solute between solvent pair, effect of number of extractions, batch and continuous extractions, some examples of liquid-liquid extraction.
- 4. **Spectrophotometric Analysis:** Ultraviolet and visible radiation, absorbance, transmittance, absorptivity, the Beer Lambert's law, limitations of Beer-Lambert's law, qualitative and quantitative analysis, stoichiometric determination of metal-ligand complexes.
- 5. Atomic Spectrometric Methods: Atomic absorption and atomic emission, absorption line width, choice of absorption line, flame emission spectrometry with emission analysis, atomic absorption spectrophotometry: principles, instrumentation and interferences, electro-thermal atomizers, sample requirements and general preparation techniques, the effect of different solvents, sensitivity, qualitative and quantitative analysis, hydride vapour generation technique, cold vapour technique, advantages and disadvantages of AAS.
- 6. Polarographic and Voltammetric Analysis: Current voltage relationship, mass transport processes, direct current polarography (DC Polarography), alternating current and pulse polarographic analysis, stripping voltammetry, applications of electrochemical sensors.

- **7.** Thermal Analysis: Thermogravimetry (TG), types of TG,instrumentation, application of TG, differential thermal analysis(DTA) working principles and applications, differential scanning calorimetry (DSC) principles and applications.
- 8. Chromatographic Techniques: Overview, retention behaviour, efficiency, selectivity, resolution, chromatographic theory, measured chromatographic parameters, evaluation methods, classification of chromatographic techniques, principles and application of liquid chromatography, ion exchange chromatography, high performance liquid chromatography and gas chromatography.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Critically evaluate data from a variety of analytical chemistry techniques and apply knowledge of the statistical analysis of data,
- (ii) Select the appropriate analytical methods to evaluate a sample.
- (iii) Explain the theoretical principles of selected instrumental methods within spectrometric/spectrophotometric method, and main components in such analytical instruments.
- (iv) Understand the underlying theoretical basis of polarographic and voltammetric analysis, thermal analysis, and chromatography.
- (v) Interpret the results of quantitative experiments and interpret the data in meaningful ways.

Books Recommended

- 1. Instrumental Methods of Analysis, H. W. Willard, L. L. Merritt Jr., J. A. Dean and F. A. Settle Jr.
- 2. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch.
- 3. Principles of Instrumental Analysis, D. A. Skoog, R. J. Holler and T.Nieman.
- 4. Analytical Chemistry, G. D. Christian.
- 5. Modern Analytical Chemistry, D. Harvey.
- 6. Analytical Chemistry, R. Kellner, J. -M. Mermet, M. Otto and H. M. Widmer Edited.
- 7. Quantitative Chemical Analysis, S. E. Manahan.
- 8. A Text Book of Quantitative Analysis, A. I. Vogel.
- 9. Analytical Electrochemistry, J. Wang.
- 10. Electrochemical methods, A. J. Bard and L. R. Faulkner.
- 11. Organic Electrochemistry, As Introduction and Guide, Henning Lund and Mannuel M. Blazer.

IA 605: Environmental Chemistry

Learning Objectives

The learning objectives of this course are to

- (i) Discuss the biotic and abiotic components of an ecosystem and describe the interactions between these components.
- (ii) Impart advance knowledge on water pollution, air pollution, marine pollution, toxicology chemistry and marine chemistry.
- (iii) Promote knowledge on water treatment, solid waste management and management of aquatic environment.
- (iv) Discuss the guidelines for healthy environment.

Course Content

1. Atmospheric Pollution and Its Effects: Natural air pollution, anthropogenic air pollution, gas-phase pollutants and photochemical smog formation, visibility, turbidity, thermal air

(Half Unit)

pollution, atmospheric deposition, acid rain, stratospheric ozone depletion, global warming, air pollution episodes, pollution exposures, impacts of pollutants on human health, health effects of respiratory air particles and PAN, health effects of noise pollution.

- 2. Water Pollution: Nature and types of water pollutants, elemental pollutants, heavy metals, metalloids, organically bound-metals and metalloids, inorganic species, algal nutrients and eutrophication, oxidants and reductants in water, organic pollutants-pesticides in water, polychlorinated biphenyls(PCBs), polyaromatic hydrocarbons(PAHs), petroleum hydrocarbons(PHs), polychlorinated bibenzodioxins(PCBDs), radionuclides in the aquatic environment.
- **3.** Humic Substances in the Aquatic Environment: Physico-chemical characteristics of humus substances in water and soil, complexation reactions of humic and fulvic acids with metal ions, detoxification, discuss some specific examples like Cu-HA complexes and biotoxicity of Cu²⁺ ion.
- 4. Water Treatment: Preliminary treatment, screening, skimming, primary treatment sedimentation, flocculation, secondary treatment trickling filters, activated sludge method, oxidation ponds, sludge disposal, tertiary treatment chlorination, wet oxidation, adsorption, reverse osmosis, electrodialysis, ion exchange, fluoridation, drawbacks of chlorine disinfection method, chloramines, ozone disinfection treatment, potassium permanganate, peroxone, ozone to H_2O_2 , ultraviolet (UV) disinfection treatment, membrane filtration for water purification.
- **5. Pollutants in Marine Environment:** Discussion on marine pollution, classification of marine pollutants, inorganics: Cd, Cu, Pb, Hg, organics, insecticides, fungicides, polychlorinated biphenyls (PCBs), polyaromatic hydrocarbons(PAHs), radioactive materials, oil pollution and its effects on marine biota, abatement of marine pollution.
- 6. Management of Solid Waste: Classification of solid wastes, disposal of bulk solid wastes, organic wastes, dried disposal of animal wastes on land, composting, sewage sludge, biogas from solid wastes, mixed urban wastes, land filling, incineration, reuse and recycling.
- 7. National Policy for the Protection of the Environment: International and National laws for the protection of the environment, Earth Summit, Environment Quality Standards, EQS, FEC and WHO guidelines for environmental health criteria.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Identify the types of air and water pollutants and deal with the various water treatment processes.
- (ii) Explore the importance of humic substances in the aquatic environment and understand the marine chemistry, importance of marine resources and marine pollution.
- (iii) Identify the toxic chemicals in the environment and their detrimental effects on human health
- (iv) Manage different aquatic environment free of pollution and manage different types of solid wastes.
- (v) Understand the safety recommendation and regulations of water and air pollution for maintaining healthy environment.

- 1. Environmental Chemistry, G. W. Vanloon and S. J. Dufty.
- 2. Environmental Chemistry, S. Manahan.
- 3. Environmental Concept of Environmental Chemistry, G. S. Sodhi.
- 4. Environmental Chemistry, A. K. Dey.
- 5. Environmental Toxicology, M. Satake, Y. Mido, M. S. Sethi and S. A. Iqbal.
- 6. Environmental Hazards, Keith Smith.
- 7. Environmental Analytical Chemistry, F. W. Fifield and P. J. Haines.

- 8. Minerals from the Marine Environment, Sir P. Kent.
- 9. Application of Environmental Chemistry, E. R. Weiner.
- 10. Toxic Metal Chemistry in Marine Environments, M. Sadiq.

IA 606: Instrumental Techniques in Chemical Analysis (Half Unit)

Learning Objectives

The learning objectives of this course are to

- (i) Give a general understanding of working principle, instrumentation and applications of advanced analytical tools for surface characterization.
- (ii) Impart knowledge on working principle, instrumentation and applications of various advanced chromatographic techniques.
- (iii) Introduce knowledge on principle and types of electrophoretic techniques and scope of separation of low and high molecular weight charged materials including DNA, protein etc.
- (iv) Acquaint the students with the modern techniques used in ultratrace analysis; such as ICP-AES, ICP-MS etc.
- (v) Give idea of automated methods in chemical analysis and computer based data processing.

Course Content

- **1.** Surface Characterization by Spectroscopic and Microscopic Methods: Principles, instrumentation and analytical application of X-ray fluorescence (XRF), particle induced X-ray emission(PIXE), and scanning electron microscopy(SEM).
- **2. Mass Spectrometry:** General principles and basic instrumental aspects of mass spectrometry, interpretation of mass spectra, principles and investigation of toxic chemicals through the application of GC-MS and LC-MS techniques.
- **3. Ion and Ion-Pair Chromatography:** Theory, columns for ion chromatography, normal and Reversed phase ion-pair chromatography, detectors and applications.
- 4. Electrophoresis: Principle of electrophoresis, paper, gel and capillary electrophoresis, opentubular electrophoresis, nature of support system and buffers, scope of separation of low and high molecular weight charged materials including DNA, protein, and enzymes etc., sample introduction and detection.
- 5. Size Exclusion and Supercritical Fluid Chromatography: Theories of exclusion and supercritical chromatography, mechanism and materials, inorganic stationary phases, application.
- 6. Ultratrace Analysis: Inductively coupled plasma atomic emission spectroscopy(ICP-AES), and inductively coupled plasma mass spectroscopy(ICP-MS) principle, instrumentation and specific applications including large scale metal scanning.
- 7. Automated Methods of Analysis: On-line flow-injection analysis, computers in analytical chemistry, data processing and graphics.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Discuss the spectra and images of target compounds through studying spectroscopic and microscopic techniques for the characterization of a surface.
- (ii) Apply various modern chromatographic techniques for the separation, identification and quantification using different detectors.
- (iii) Understand the underlying principles, instrumentation and applications of mass spectrometry (MS), GC-MS, LC-MS.
- (iv) Apply different electrophoretic and ultratrace analytical techniques.
- (v) Handle automated machine and computer based data processing for mass scale analysis.

Books Recommended

- 1. Principles of Instrumental Analysis, D. A. Skoog, F. J. Holler and T. A. Nieman.
- 2. Analytical Chemistry, G. D. Christian.
- 3. Modern Analytical Chemistry, D. Harvey.
- 4. Analytical Chemistry Handbook, J. A. Dean.
- 5. Fundamentals of Analytical Chemistry, D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch.
- 6. Analytical Chemistry Principles, J. H. Kennedy.
- 7. Chemical Analysis, H. A. Laitinen.
- 8. Quantitative Chemical Analysis, D. C. Harris.

IA 607: Bioinorganic Chemistry

(Half Unit)

Learning Objectives

The learning objectives of this course are to

- (i) Promote knowledge on bioelements and their compounds.
- (ii) Deliver knowledge on biomolecules like metalloporpyrin and their role in biological system and natural chemistry.
- (iii) Provide advance knowledge of the role of different metalloenzymes in catalytic reactions in biological system.
- (iv) Give concepts of beneficial and toxic effects of certain metals in certain forms and doses on life and how to detox heavy metals toxicity.
- (v) Acquainted with medicinal inorganic chemistry.

Course Content

- 1. Metals in Biological Systems: Elements in the biosphere, classification of elements as extracellular, organelles and cytoplasmic, roles of Na, K, Mg and Ca in human, sodium-potassium pump, cyclic enzyme reactions in sodium pumping, ATP and eversion mechanism, selectivity of Na-K in eversion, calcium biochemistry.
- 2. Oxygen Transport: Metalloporphyrin and the formation of hemoglobin and myoglobin, structures of these two blood carriers, the O₂ binding site in hemoglobin, magnetic and structural properties of transient Fe-O₂ system in hemoglobin, properties of Fe and Cu carriers of O₂, the coordination environments of hemoglobin and myoglobin, the t_{2g}⁴ and e_g² and t_{2g}⁶ configurations of Fe and the O₂ binding at the Fe sites, the pi-acceptor ligands CO, NO, CN, N³⁻, RCN and SCN competing with O₂ for the Fe atom, the O₂ saturation curves, models O₂ binding and the concept of artificial blood.
- **3. Metalloenzymes:** Classification of metalloenzymes in human, structure-function relationship of the metalloenzymes, the mechanism of zinc carboxypeptidase and zinc carbonicanhydrase in protein hydrolyses and CO₂ conversion to HCO₃ in human, redox catalysis, the mediator enzymes, cytochrome P-450 enzymes and its mechanism, the nitrogen fixation.
- 4. Metals in Medicines: Clinical functions and metal requirements, cisplatin and auranofin, metal deficiency and diseases, anemia and iron, causes and consequences of zinc deficiency, toxic effects of metals copper overload and Wilson's disease, iron toxicity, mercury toxicity and bacterial resistance, cadmium and lead toxicity, lithium and mental health, gold and arthritis, metallocenes and their halides, metals as carcinogens, anticancer drugs, plutonium a consequence of nuclear age, magnetic resonance imaging, radiodiagnostic agents.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Acquire knowledge about biological systems, bioelements and their compounds.
- (ii) Describe the operation of the sodium potassium pump.
- (iii) Identify and explain the different classes of metalloenzymes and their catalytic role in biological processes.
- (iv) Recognize beneficial and toxic effects of certain metals in certain forms and doses on life and how to detox heavy metals toxicity.
- (v) Understand the role of metals in medicines.

Books Recommended

- 1. Bioinorganic Chemistry, Bertini, Gray, Lippard and Valentine.
- 2. Advanced Inorganic Chemistry, F. A. Cotton and G. Wilkinson.
- 3. Inorganic Chemistry, J. E. Huheey.
- 4. Inorganic Chemistry, D. F. Shriver, P. W. Atkins and C. H. Langford.
- 5. Inorganic Chemistry, G. L. Miessler and D. A. Tarr.

IA 608: Chemical Crystallography and Solid State Chemistry (Half Unit)

Learning Objectives

The learning objectives of this course are to

- (i) Deepen and widen students' knowledge on the structures of solids.
- (ii) Achieve fundamental knowledge on X-rays, X-ray diffraction, Bragg's equation for X-ray diffraction, uses of powder and single crystal X-ray diffraction.
- (iii) Aware about the different large single crystal growth methods.
- (iv) Introduce the concept of relating structure to physical properties.
- (v) Provide basic knowledge of superconductivity.

Course Content

- 1. X-Ray and Crystals: X-rays, properties of X-rays, diffraction of X-rays by crystals, reciprocal lattice, Bragg's law in reciprocal lattice, sphere of reflection, limiting sphere, crystal growth, techniques of single crystal growth, choosing a crystal, diffractometry, crystal mounting, measurement of crystal properties, data collection, integrated intensities, unique data, the indexing of reflection and determination of space groups.
- 2. Data Reduction and the Phase Problem: Lorentz and polarization corrections, absorption and extinction corrections, radiation damage correction, scaling, the structure factor, Friedel's law, the Fourier transformation, the electron density equation, the phase problem.
- **3.** Solution of the Phase Problem: The Patterson function, Harker lines, Harker planes, heavy atom method, direct methods, unitary structure factor, normalized structure factor, probability method, tangent formula, symbolic addition, modern developments.
- 4. Completing the Structure: Observed structure factor, calculated structure factor, F_o synthesis, ΔF synthesis, identification of atom types, location of hydrogen.
- 5. Refinement of Structures: Matrix manipulations, the principles and practices of the method of least squares, series termination error, refinement by ΔF synthesis, refinement against F_o^2 , weighting function, goodness of fit parameter, residual indexes, restrained refinements.
- 6. Derived Results: Bond lengths, bond angles and torsion angles calculations, calculations of their esd's, correlation coefficients, thermal motions, anomalous scattering and its effects, absolute configurations.
- 7. **Powder Diffraction Techniques:** The powder method principles and uses, Guinier focusing camera, the powder diffractometer, measurement of d-values, refinement of unit cell parameters, indexing of powder patterns, and structure determination from powder patterns.

- 8. Synthesis of Solid Materials: Reaction types, quality criteria and assessments, sol-gel technique, thin film preparation, chemical transport, thermodynamic of solid state reactions, liquid crystals, classifications of liquid crystals and their possible phase transitions.
- **9. Properties of Solid Materials:** Phase transitions, classifications of phase transitions, stable and metastable phases, representation of phase transitions on phase diagram, electrical conductivity of inorganic solids, dielectric materials, ferroelectricity, pyroelectricity and piezoelectricity, structure and magnetic property relation of transition metal oxides, perovskites, spinel and illmenites.
- **10. Superconductors:** Superconductivity, theories of superconductivity, applications, recent development of superconducting materials.

Learning Outcomes

Upon completion of this course, the students will be able to

- (i) Explain the principles concerning crystal structures of solid.
- (ii) Understand the principle of X-ray generation, X-ray powder diffraction by crystals and their interpretation and can demonstrate the elementary idea about the single crystal X-ray diffraction.
- (iii) Synthesize large single crystal of solids.
- (iv) Present the properties of various solid materials.
- (v) Describe the phenomenon of superconduction of materials.

- 1. X-Ray Structure Determination A Practical Guide, G. H. Stout and L. H. Jensen.
- 2. Crystal Structure Analysis- A Primer, J. P.Glusker and K. N. Trueblood.
- 3. Structure Determination by X-ray Crystallography, M. F. C. Ladd and R.A. Palmer.
- 4. X-Ray Methods Analytical Chemistry by Open Learning, C. Whiston.
- 5. Solid State Chemistry and Its Applications, A. R. West.
- 6. Inorganic Solids, D. M. Adams.
- 7. An Introduction to Crystal Chemistry, R. C. Evans.