UNIVERSITY OF PUNE

Department of Chemistry

M.Sc. INORGANIC CHEMISTRY (Semester III and IV) 2014-2015

	Course No.	Compulsory courses	Total credit per semester
Sem.-III	CHI-320	Physical methods of coordination compounds and Bio-inorganic chemistry	5
	CHI-321	Inorganic reaction mechanism and Photochemistry	5
	CHI-322	Organometallic chemistry and Homogeneous catalysis	5
	CHI-323	Frontier's in material science and Analytical techniques for solids	5
Sem.-IV	CHI-420	Inorganic polymers, clusters and Heterogeneous catalysis	5
	CHI-421	Solid state chemistry of Inorganic Materials	5
	Optional Course (Any one)		
	CHI-423	Industrial inorganic chemicals and medicine chemistry	5
	CHI-425	Advanced Techniques in Inorganic chemistry	5

Practical courses

Course No.	Practicals (Semester III)	Credits
CHI -328	Classical Inorganic Chemistry Practicals –I	4
CHI -329	Instrumental Inorganic Practicals -II	4
	Practicals (Semester IV)	
CHI-428	Project Work	7

Department of Chemistry

University of Pune

M. Sc (Inorganic Chemistry) Syllabus under the credit system at Department of Chemistry, University of Pune, Pune 411007 is effective for the academic year 2014-15.

The M. Sc. course in Chemistry for two years will consist of 100 credits. Each semester will run for 15 weeks. We will have 70 credits for theory and 30 for practicals and project work.

The proposed structure for M. Sc. Semester III-IV (Inorganic Chemistry) is the following:

Semester 3:

CHI-320: Physical methods of coordination compounds and Bio-inorganic chemistry (5 credits &60 lectures)

CHI-321: Inorganic reaction mechanism and Photochemistry (5 credits & 60 lectures)

CHI-322: Organometallic chemistry and Homogeneous catalysis (5 credits & 60 lectures)

CHI-323: Frontier's in material science and Analytical techniques for solids (5 credits&60 lectures)

Semester 4:

CHI-420: Inorganic polymers, clusters and Heterogeneous catalysis (5 credits &60 lectures)

CHI-421: Solid state Chemistry of Inorganic Materials (5 credits &60 lectures)

OPTIONAL (Any one)

CHI-424: Industrial inorganic chemicals and medicine chemistry (5 credits &60 lectures)

CHI-425: Advanced Techniques in Inorganic chemistry(5 credits & 60 lectures)

Practicals:

SEMESTER III

CHI-328: Classical Inorganic Chemistry Practicals –I (4 credits, ~7.5 weeks)

CHI-329: Instrumental Inorganic Practicals-II (4 credits, ~7.5 weeks)

SEMESTER IV

CHI-428: Project Work (7 credits, ~13.5 weeks)

CHI-320:Physical methods of coordination compounds and Bio-inorganic chemistry- II(5 credits and 60 lectures)

Section I:Physical methods of coordination compounds (30 Lectures)

1. Theoretical and Practical aspects of Magnetism in Coordination Complexes [16]

Determination of state functions of R-S terms of d^2 and p^2, transition metal ions.

Derivation of Van Vleck's expression and μ_{S+O} formula, Quantization of orbital contribution in d^1 ion and quenching in cubic crystal field.

Magnetic moments based on crystal field ground term, Perturbation Theory and its application, Spin orbit coupling operator for magnetic susceptibility and magnetic moment of T terms and A, E terms .

Anomalous magnetic moments in magnetically dilute and concentrated system in various symmetrical environments of coordination complexes.

2. Electron Paramagnetic Resonance Spectroscopy (EPR) [7]

Theory and Instrumentation of EPR.

Spin Hamiltonian, Isotropic and anisotropic EPR spectra, Magic Pentagon rule.

Applications of EPR spectroscopy: (1) Structural determination of Inorganic complexes. (2) Applications metalloproteins, Fe, Cu.

3. Nuclear Quadrupole Resonance (NQR) [3]

i) Principle selection rule for NQR

ii) Factos for splitting of quadruple energy levels in NQR

iii) Application of NQR: Structural information from NQR

4. Cyclic Voltammetry (CV) [4]

Principle of Cyclic Voltammetry, typical features of CV curve, CV advantages and disadvantages.

Instrumentation

Electrolytes

Application of CV technique (a) Inorganic Compounds (b) Organic Compounds.

Books:

"Magnetism and Transition Metal Complexes", F. E. Mabbs and D. J. Machin (Chapman and Hall) London(1973).
"Introduction to Magnetochemistry", A. Earnshaw, Academic Press, (1968).

Elements of Magnetochemistry, R. L. Dutta and A. Syamal, Affiliated East/West Press Pvt. Ltd. 2007.

"Physical Methods in Chemistry", R. S. Drago (2nd Edition) (1977).

"Electrochemistry for Chemists", D. T. Sawyer, A. Sobkowak, J. L. Roberts Jr. 2nd Edition, John Wiley, Inc. New York, 1995).

Section II:Bioinorganic Chemistry **(30 Lectures)**

(1) Recapitulation of Biological Roles of Metals & Ligands (3L)

Structural Information

Metal Activity, Specificity & Selectivity

Biochemical Evolution of Metals in Biological System

(2) Biological Chemistry of Iron (7L)

Transport of Iron

Hemoglobin & Myoglobin (including their model compounds)

Storage & Transport Proteins of Iron viz,. Ferritin & Transferrin

Cytochromes

Iron-Sulfur Proteins

(3) Biochemistry of Cobalt (3L)

B12 Coenzymes and Model compounds

Actions of Cobalmins&Cobinamides

Adenosylcobalmin as a Coenzyme

Ribonucleotidereductase

Methylcobalmin as cofactor

(4) Biological Chemistry of Copper (7L)

Type I, II & III

Blue Copper Proteins (PlastocyaninsAzurins& Blue Oxidases)

Models of Blue Copper Compounds

Non-blue copper proteins e.g. Tyrosinase, Galactose Oxidase, SOD etc.

(5) Biological Chemistry of Molybdenum (3L)

Antagonism between Cu & Mo

Mo cofactors

ESR Spectra features

Hydroxylase Enzymes

(6) Biological Chemistry of Vanadium and Chromium (2L)

Vanadium proteins including bromoperoxidases

Glucose Tolerence Factor

Vanadium Nitrogenase

(7) Biological Chemistry of Zinc (5L)

a) Carboxypeptidase and Carbonic anhydrase enzymes

Books :

Bioinorganic Chemistry : A Short Course –Rosette M.Roat-Malone, Wiley Interscience, 2002.

Biological Inorganic Chemistry –An Introduction, Robert Crichton, Elsevier Science, 2007

The Biological Chemistry of the Elements- The Inorganic Chemistry of Life

J.J.R.Frausto da Silva and R.J.P.Williams Clarendon Press, Oxford,1991.

CHI - 321: Inorganic Reaction Mechanism and Photochemistry (5 credits and 60 lectures)

Section I: Inorganic Reaction Mechanism (30 lectures)

1. Types of Mechanisms: Basic concepts as stability and lability, stability constants; HSAB principle, chelate effect,Macrocyclic effect; Ligand transfer and electrontransfer reactions in coordination compounds, Intimate and stoichiometric mechanismof ligand substitution.

2. Substitution in square planar complexes: trans effect, trans series, applications of trans effect.

3. Substitution in octahedral complexes: S_N1, S_N2 S_NICB mechanisms, racemization in coordination compounds, stericeffects on substitutions.

4. Electron Transfer reactions: Potential energy diagrams as a conceptual tool, Marcus equation, Types of and factors affecting electron transfer reactions.

5. Inner and Outer sphere reactions.

Books:

1. "Comprehensive Coordination Chemistry", Pergamon G. Wilkinson, R. D. Gillard andJ. A. McCleverty, , Vol. 1, pp281-322, 331- 379, 385-411, 415-458 (Chapt. 7.4) and 463-471, (1987).

2. "Inorganic Chemistry", D. F. Shriver, P. W. Atkins and C. H. Langford, 2nd edn. Oxford, Chapt.15, p.559, (1994).

References:

"Inorganic Chemistry – Principles of Structure and Reactivity", J. E. Huheey, E. A. Keiter and R. L. Keiter, 4thedn. Harper Collins College Publ. New York, Chapt.13, p.537-76, (1993).

"Mechanism of Inorganic Reactions in Solution – An Introduction", D. Benson, McGraw – Hill Chapt.15, p.465, (1968).

"d- and f- block Chemistry", C. J. Jones, p. 78, 85 and 122. Tutorial Chemistry Texts, E. W. Abel (Ed.), Royal Society of Chemistry, Cambridge (2001).

"Basic Inorganic Chemistry", F. A. Cotton and G. Wilkinson, Wiley Eastern Ltd., NewDelhi p.154, (1990).

Section II:Inorganic Photochemistry and Reaction types (30 lectures)

(1) Photochemical Reactions: Prompt and delayed reactions, Quantum yield, Recapitulation of fluorescence and phosphorescence. Photochemical reactions by irradiating at d-d and charge transfer bands. Transitions in metal-metal bonded systems. Photochemical reactions involving chlorophyll. Kinetics of excited state processes. (8)

(2) Photophysics of transition metal complexes in solution: Types of excited states and electronic transitions, absorption and emission bands, photochemical reactivity, polynuclear metal complexes. (2)

(3) Chemical Actinometry: Ferrioxalateactinometer , Photochromic actinometer , Reinecke's salt actinometer, Uranyl oxalate actinometer, Other actinometers. (2)

(4) Other Reaction types: Oxidative addition, Reductive elimination reactions, Methyl migration and CO insertion reactions. (2)

(5) Reactions of coordinated ligands:

(i)Non-chelate forming reactions: Reaction of donor atoms(Halogenation of coordinated N atoms, Alkylation of coordinated S and N atoms, Solvolysis of coordinated phosphorus atoms). Reactions of non-donor atoms (nucleophilicbehaviour of the ligand, electrophilic bahaviour of the ligand).

(ii) Chelate ring forming reactions: (reactions predominantly involving thermodynamic templateeffects, reactions predominantly involving kinetic affects).

(iii) Chelate modifying reactions (12)

(6) Isomerization reactions of thermal and photochemical types involving four coordinated and six coordinated metal complexs. Bailar and ray Dutta twist. (4)

Books:

Inorganic Chemistry, D.F.Shriver, P.W.Atkins and C.H.Langford, Oxford, 2nd. edn. 1994.

An Introduction to Inorganic Chemistry by K.F.Purcell and J.C.Kotz, Saunders 1990, Chapter 14.

Comprehensive Coordination Chemistry, Vol.1. G Wilkinson (Ed) Wiley, New York, 1967.

Inorganic Chemistry by J.E.Huheey, E.A.Keiter and R.L.Keiter 4th edn. Harper Collins, 1993

Mechanisms of Inorganic Reactions, by C.F.Basolo and R.G.Pearson, Wiley, New York, 1967.

CHI -322: Organometallic Compounds & Homogeneous Catalysis (5 credits & 60 lectures)

Section I:Organometallic Chemistry (30 lectures)

1. Introduction, definition and scope of organometallic Chemistry (2)
Valence electron count
18 and 16 electron complexes

2. d-block carbonyls : (5)
coordination modes
characterization
synthesis
reactions
carbonyl metallates
ligands related to CO

3. σ-organyls : Synthesis, bonding, Properties and applications of (5)
alkyls
aryls
alkenyls
acyl
alkynyls

4. Metal-Carbon multiple bonded compounds : Synthesis, bonding, Properties and applications of (2)
carbenes
carbines

5. Π-complexes (2)
alkenes
d—and polyenes

6. η^n-C_nR_n carbocyclic polyenes : Synthesis, bonding, Properties and applications of (6)
allylsη^3-C_3R_5
pentadienylsη^5-C_5R_7
cyclopropenylsη^3-C_3R_3
cyclobutadienesη^4-C_4R_4
cyclopentadienylsη^5-C_5R_5
arenas η^6-C_6R_6
cycloheptatrienylsη^7-C_7R_7
cyclooctatetraenes.

7. Metal-Metal Bonds and Transition Metal atom clusters (2)

8. Transition Metal organometallic intermediates in organic synthesis (6)
nucleophiles
electrophiles
migration
protective reagents

Books:

1. Inorganic Chemistry 3rd edn. D.F.Shriver and P.W.Atkins, Oxford University Press, 1999, Chapter 16.
2. Organotransition Metal Chemistry, Anthony F.Hill, Royal Society of Chemistry,Tutorial Chemistry Text, 2002. Chapters 1 to 7.
3. Organometallics: A concise Introduction, Ch.Elshebroicn and A Salzer, VCH, Chapters 12 to 16.

Organotransition Metal Chemistry: Applications to Organic Synthesis, S.G.Davies, Pergamon 1982.

Section –II : Homogeneous Catalysis (30 lectures)

(1) Introduction to Catalysis, basic principles: Interplay of Kinetics and thermodynamics in chemical reactions and the role of catalysts. Definition of activity, selectivity in catalysis; homogeneous vs. heterogeneous catalysis; importance of homogeneous catalysis in the synthesis of high value chemicals.

(2) Characteristics of central metal ions and influence of attached ligands on catalytic activity; important properties of ligands, elementary steps: Important reaction types: Oxidative addition and reduction; elimination, insertion (migratory) reactions, β-hydride elimination, nucleophilic attack, catalytic cycle; catalytic intermediates and their identification through spectral techniques (IR, ESR, NMR….).

(3) What are the reactions that olefins undergo? Hydrogenation of olefins; Wilkinson's catalyst; catalytic cycle. Asymmetric hydrogenation (Enantio-slective hydrogenation).

(4) Other reactions of alkenes: Isomerization, dimerization, oligomerization, hydrocynation and metathesis reactions: Common reactive intermediates. Examples of Shell higher olefin process, DuPont Adiponitrile process.

(5) Carbonylation reaction: methanol to acetic acid process and the catalysts employed in BASF and Monsanto processes. Carbonylation of alkynes and other substrates for making industrially important chemicals.

(6) Hydroformylation: Cobalt and Rhodium complexes, the role of phosphine ligands in regio selective formation of linear aldehydes. Markovnikov and anti-Markovnikov addition and mechanisms.

(7) Polymerization: Catalytic cycle for alkene polymerization; Metallocene catalysts, structure, special features and advantages of metallocene catalysts; mechanism of polymerization and stereocontrol by metallocene catalysts.

(8) Oxidation reactions; Wacker oxidation, metal-catalyzed liquid phase oxidation (cyclohexane, p-xylene); epoxidation of propylene; Oxo complexes as homogeneous oxidation catalysts; mechanism of oxidation reactions.

(9) Hydrosilylation :platinum catalyst , Asymmetric palladium catalyst, Rhodium Catalysts for asymmetric ketone reduction .

(10) Asymmetric Catalysis: General features of chiral ligands and complexes; Mechanisms and Catalytic cycles in hydrogenation, isomerization, epoxidation and catalytic reactions of C-C bond formation

Books :

Homogeneous Catalysis: The Applications and Chemistry of Catalysis by Soluble Transition Metal Complexes, G.W. Parshall and S.D. Ittel, Wiley, New York 1992

Applied Homogeneous Catalysis with Organometallic Compounds, Vols. 1 & 2, edited by B. Cornils and W.A. Herrmann, VCH, Weinheim, New York, 1996

Homogeneous Catalysis: Mechanisms and Industrial Applications, S. Bhaduri and D. Mukesh, Wiley, New York, 2000

Homogeneous Catalysis: Understanding the Art, P.W.N.M. van Leeuwen, Kluwer Academic Publishers, 2003

CHI-323: Frontier's in material science and Analytical techniques for solids (5 credits & 60 lectures)

Section IFrontier's in material science (30 lectures)

1. The Structure of solids: (5 L)

Voids in closest packings; Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX_2, spinel structure andperovskite structure.

2. Crystal Defects and non-stoichiometry: (6L)

Classification of Defects: subatomic,atomic and lattice defects in solids; Thermodynamics of vacancy in metals; Thermodynamics of Schottky defects in ionic solids ; Thermodynamics of Frenkel defects in silver halides; Calculation of number of defects and average energy required for defect, Other examples of defect structure; Non-stoichiometry and its classifications.

3. Diffusion in solids: (4L)

Mechanism of Diffusion; Ficks first law and second law of diffusion in solids; Kirkendal effects in solids.

4. Phase Transformations in Solids: (5L)

Gibbs Phase rule;time scale of phase changes; Phase diagram of binary system; types of phase transitions.

5. Solid State reactions and Crystal Growth (5L)

Classification of solid state reactions and their kinetics and mechanisms; thermal decomposition reaction; law governing nucleation;Growth of nuclei; Reaction between two solids;Improving the reactivity of solids;Zone refining method;Crystal growth.

6. Preparative method of solids: (5L)

Introduction, Ceramic method, microwave synthesis, Sol-gel method, Precursor method, Hydrothermal method, Chemical vapour deposition (CVD) Method,Chemicalvapour Transport, Choosing a method for solids.

Books:

Solid-State Chemistry an Introduction (2^{nd} Edition) – Lasley Smart and Elaine Moore (Chapman & Hall 1996)
Solid State Chemistry- D.K.Chakraborty (New Age International Pvt.Ltd.New Delhi, 2000)
Introduction to Soilds-L.V.Azaroff (tata McGraw Hill Publication Ltd. New York)
Principles of the Solid State-H.V.Keer (Wiley Eastern Ltd.New Delhi, 1994)
Solid state Chemistry –N.B.Hannay (Prentice Hall, New Jersey, 1967)

Section II : Analytical techniques for solids **(30 L)**

1. Thermal Analysis: (10L)

a) Thermogravmetry (TGA): Definition, Types of TGA, Instrumentation, Information from TGA Curve; Factors affecting TGA curves (instrumental as well as characteristics of sample factors); Application of thermogravimetry; Calculation of percent decomposition and composition of compounds; Limitation and Advantages of TGA.

b) Derivative thermogravimetry(DTG) and its advantages

c) Differential Thermal Analysis (DTA) : Definition; Theoretical Basis of DTA;Instrumentation for DTA apparatus; Factors affecting the DTA curve; Application of DTA; Advantages and disadvantages of DTA.

d) Differential Scanning Calorimetry (DSC) : Definition ; Comparison of DTA and DSC techniques; Istrumentation of DSC, Factors affecting DSC curves.

2. X-ray Diffraction: (10L)

a) X-ray powder diffraction (XRD):

X-ray source, Diffraction of X-rays,X-ray powder diffraction, Instrumentation and use of standards, identification of compounds using powder diffraction.The importance of intensities, Absences due to lattice centring;Determination of unknown cubic crystal structure by $\sin^2\theta$ method; Parameter to be determined from XRD: Qualitative analysis; Quantitative analysis-percent crystallinity, Crystallite size, surface area, unit cell dimension.

b) Single crystal X-ray diffraction:

Solving single crystal structures; refining a structure, X-ray crystal structures in the literature.

3. X-ray Photoelectron spectroscopy(XPS): (5L)

Introduction and basic theory; Instrumentation;Sample selection and preparation, Spectral analysis; XPS imaging.

4. X-ray Fluorescence spectroscopy (XRF) (5L)Introduction and basic theory; Instrumentation, spectral analysis; Analytical information and applications.

Books :

Thermal Analysis-Wendland

Instrumental Methods of Analysis-G-Chatwal and S. Anand (Himalaya Publication;1988)

Catalysis: Principles & Applications-B.Viswanathan,S.Savasankar and A.V.Ramaswamy (Narosa Publication; 2004). (For XRD part)

Solid State Chemistry: An Introduction-Lesley Smart and Elaine Moore (2nd Edition, Chapman and hall, 1996).

Crystallography and its applications-L.S.DentGlasser (Van Nostrand, 1977)

Handbook of Applied Solid State Spectroscopy-D.R.Vij (Springer Science, 2006).

Optical Properties and Spectroscopy of Nanomaterials-Jin Zhong Zhang (World Science Publication, 2004).

Solid Chemistry: techniques-A.K.Cheetham and P.Day (oxford University Press, 1987).

Crystal Structure Analysis- M.J.Buerger(John Wiley, 960).

Physical Methods for Chemists-R.S.Drago(2nd Edition, Saunders).

Other Books:

Element of X-ray Diffraction-B.D.Cullity (1967)

The Synthesis and Characterization of Inorganic Compounds-W.L.Jolly (Prentice Hall, 1970).

Synthesis and Techniques in Inorganic Chemistry-R.J.Angelias (2nd Edition, Saunders, 1977).

Structural Methods in Inorganic Chemistry –E.A.V.Ebsworth,D.W.H.Rankin and S.Cradock (Blackwell Scientific Publication, 1987).

Semester IV

CHI-420 Inorganic polymers, clusters and Heterogeneous catalysis (5 credits and 60lectures):

Section I : Inorganic Polymers (30L)

1. Inorganic polymers: Overview of polymers, Classification schemes.

2. Inorganic polymer characterization: Average molecular masses (M_n, M_w) and degree of polymerization, method of characterizing average molecular masses, determination of thermal parameters, viscoelasticity measurements , crystallization characterization.

3. Bridge between small and finite molecules , Homopolar inorganic polymesr, Heteropolar inorganic polymers, Polyphosphazenes, Polysiloxanes,Polysilanes and Boron based polymer, Phosphorous based polymer , Sulphur containing polymer, Metal coordination polymers.

4. Pre-ceramic Inorganic polymers: Silicon carbide, Boron nitride, Aluminiumnitride, Phosphorous nitride.

5. Applications of Inorganic Polymers: Metal containing polymer for medical purposes, Inorganic polymers as a catalysts, Luminescent Inorganic polymers.

6. Metal clusters: Metal-metal bonds, Framework bonding in metal clusters, Synthesis of metal clusters. Types of clusters viz. carbonyl clusters, Halide type clusters, Boron clusters and their applications.

Text book

1. I. S. Butler and J. F. Harrod, Inorganic Chemistry – Principles and Applications,

2.The Benjamin/Cummings Publishing Co., Inc., Redwood City, California (USA)(1989) Chapt. 15 to 17, pp 441-503.

3. Ranald D. Archer, Inorganic and organometalic polymers, A John Wiley and Sons, Inc. publication (USA) 2001

References

1. N. H. Ray, Inorganic Polymers, Academic Press (1978).
2. A.F. Wells, Structural Inorganic Chemistry, 5th edn., Oxford (1984).
3. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, University Science Books, Mill valley, California (USA) (1994).

Section II: Heterogeneous Catalysis (30 Lectures)

1.The Descriptive Chemistry of Heterogeneous Catalysis: (6L)

Definition of Catalysis, classification of catalytic systems, classification of solid catalysts, Adsorption of molecules at the solid surfaces, Adsorbed states of molecules on metals, potential-energy curves for adsorption, descriptive chemistry of chemisorption on metals, chemisorption and catalysis by metals-quantitative aspects, catalysis by unsupported and supported bimetals, Adsorption and catalysis on semiconducting oxides, selective oxidation of hydrocarbons. Different types of reactors.

2. Zeolite Compounds and Heterogeneous Catalysis: (8L)

(a) Introduction to porous materials:Classification into micro-, meso- and macro porous materials, the origin of pores and its significance, distinction from condensed materials.

(b) Zeolites:Definition, natural and synthetic zeolite or aluminosilicates, the primary and secondary building blocks, final framework structures, Lowensteins rule, sodalite and other structures, Nomenclature: Atlas of zeolite; structural distinctions, Novel zeolites, examplels of small, medium, large and extralarge pore zeolites; general properties and and application of molecular sieves.

(c) Characterization of zeolite: SEM,TEM and other techniques; spectral techniques: FT-IR and solid-state NMR; sorption capacity, surface area by BET method, pore volume and pore structure, the origin of Brönsted and lewis acidity in zeolites, the number and the strength, techniques for the estimation of acidity: adsorption of bases and IR spectra, temperature programmed desorption of bases.

3. Photocatalysis using semiconducting oxides (3L)

Introduction, definition of photocatalysis, basic principles involved in photocatalysis, mechanism of photocatalysis, application of photocatalysis in various fields such as water remediation, air cleaning, etc.

4. Heterogeneous catalysis by intercalation compounds: (3L)

General aspects of interstial compounds of Graphite, structural aspects of graphite intercalation compounds, physical and chemical properties, catalytic reaction.

5. Heterogeneous catalysis by perovskite- related oxides: (4L)

Solid state properties of perovskite like oxides, Relation of solid state and catalytic properties perovskites.

6. Immobilization of transition metal: complex catalysts on Inorganic support (i.e Anchored Catalysts) (3L)

General aspects of transition metal complexes as homogeneous catalysts (i.e.heterogenizing); Preparation of organometalic catalyst anchored to silica: preparation of metal ligand complex followed by Anchoring, Preparation of metal complex from previously Anchored phosphines.

8. Application of Heterogeneous catalysis: (3L)

Food industry, fine chemicals, petroleum industry, petrochemical industry, heavy inorganic chemicals, catalysis in atmospheric pollution (at least one example of application should be discuss).

Books:

Heterogeneous catalysis principles and application, G.C.Bond.

Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen (Elseviver Pub. Amsterdam, 2001)

Catalysis: Principles and Applications, B.Vishwanathan, S. Sivasankar and A.V.Ramaswamy (Narosa Pub. House, New Delhi, 2004)

Advanced material in catalysis, James J. Burton and Robert L.Garten (Academic press, Newyork, 1977)

CHI-421: Solid state chemistry of Inorganic Materials (5 Credit, 60 Lectures)

Section I :(30 Lecture)

1. Introduction to Nano-Materials

Definition and types of nano-materials, why are nano-particles are important? size dependent properties, various techniques for making nano-materials, application of nano-materials.

2. Electronics and optical materials

Electronic Materials and their application: Origin of valence and conduction bands in solids, classificationof solids into metals, semiconductor and insulator; type of semiconductivity; mobility of charge carriers, temperature dependent conductivity, some examples of semiconducting materials. Application of semiconducting devices; Metal-Metal junction (i.e. Peltier and Seebeckeffects), diodes (p-n junctions), transistors (n-p-n junctions), metal-semiconductor junction.

Optical materials and their properties: Photonic devices, Photoluminescence, Crystalline Lasers

3. Magnetic Materials

Atomic magnetismand solids, type of magnetic materials, the exchange interactions, hysteresis loops and their classification, calculationof magnetic moment from saturation magnetization, magnetic domains. Examples off magnetic materials: soft and hard ferrites, i.e. structure and magnetic interactions in spinels, garnets, hexagonal ferrites. Application of magnetic materials

4. Superconducting Materials

Definition of superconductivity, Critical temperature (Tc), Critical field, Bardeen – Cooper - Schrieffer (BCS) theory, properties and classification of superconducting compounds, High Tc superconductivity, Examples of superconducting materials: Structure of $YBa_2Cu_3O_{7-\delta}$ oxide, Fullerenes, intermetallic superconductors, synthesis of superconductors. Application of superconducting materials.

Section II:(30Lecture)

1. Ceramic Materials

Classification of ceramics, dielectric properties and polarizationproperties of ceramics, piezo-, pyro- and ferro-electric effect of ceramics, sol-gel processing of ceramics. Examples and application of ceramics: oxides, carbides, borides, nitrides.

2.Composite Materials

Definition, glass transition temperature, fibers for reinforced-plastic composite materials (i.e. glass fibers, carbon fibres, and aramid fibers); concrets and asphalt materials. Application of composite materials.

3. Cementitious Materials

Difference between Blended and Non-Portland cements; Non-portland cements; high alumina cements, calcium sulfoaluminate cements, phosphate cements.Chemicals in cement hydration; hydration process, set retarders and accelerators, plasticizers, slip-casting processing. Application of cementitous materials.

4.Bio-materials

Definition of biomaterials and biocompatibility;, Type of bio-materials: Metallic materials, Biopolymeric materials, Bioceramic materials (dense hydroxyapatite ceramics, bioactive glasses,and bioactive composites); Basic requirement of bone implants; Coating of hydroxyapatite on porous ceramics; Biomaterials in tissue attachments; Application of Biomaterials

Books:

Introduction to Solids - L. V. Azaroff (Tata MaGraw Hill)

Materials Science and Engineering – V. Raghavan (2^{nd} Edition 1980)

Elements of Materials Science and Engineering – Van Vlack (5^{th} Edition, Wiley 1988)

Nature and Properties of Engineering Materials – Z. D. Jastrazebski (John Wiley Sons, 1989)

Principles of Materials Science and Engineering – William F. Smith (Wiley, 1991)

Insight into Speciality Inorganic Chemicals – David Thompson (The Royal Society of Chemistry, 1995 chapter 13 and 14)

OPTIONAL COURSES (any one)

CHI-424:Industrial inorganic chemicals and medicine chemistry(5 credits; 60 Lectures)

Section I: Inorganic Application in Industry (30L)

a.Inorganic Chemicals as metallic Corrosion Inhibitors: (6L)

Introduction, Principles of corrosion inhibitors, corrosion as an electrochemical process, Practical aspects of corrosion inhibition,Anion inhibitor properties in neutral electrolytes,some application of corrosion inhibitors (cooling water circulation-once through and open systems,engine radiation & cooling systems,central heating system,refrigeration plants and high chloride systems, water for steam raising,corrosion inhibitors for paint coating).

b. Industrial gases: (6L)

Introduction, Separation of gases from air,Hydrogen,Carbon dioxide , Carbon monoxide , Oxygen, Acetylene , Sulphur dioxide , Nitrous oxides .

c. Chemical explosives and propellants: (6L)

Introduction, Potential energy of explosives , Properties of explosives, Manufacture of explosives , Explosives made by nitration, Dynamite , Commercial high explosives containing no nitroglycerine , Initiating devices, Sporting and military explosives , Disruptive explosives for military use, Handling and storage of explosives.

d. Metal finishing technology: (4L)

Fundamental considerations, Electrodepositions of Copper , Nickel, Gold, Silver, Tin and Tin alloys for Lead free solder, Elctorodeposition of Chromium , Elctorodeposition of semiconductors , Elctoroless deposition of Copper and Nickel, Environmental aspects of electrodeposition , Ionic Liquid treatments for enhanced corrosion resistance of Magnesium based substrates.

e. Safety consideration in chemical process industries: (5L)

Introduction , Concern for chemical safety , Hazards and their control in petrochemical industries , Hazards and their control in petroleum refineries and LPG boiling plants , Hazards in storage , Handling and use of chemicals, Chemical storage- safety issues, Observations related to safety aspects , Specific recommendation for hazard control and improved plant safety, Chemical plant safety- from concept to decommissioning.

f.Green Chemistry : (3L)

Introduction, Designing a Green synthesis, Basic Principles of Green Chemistry, Green Chemistry in Day-to-Day life, Green Chemistry in sustainable development.

1. **Books:**

2. Handbook of Industrial Chemistry,Vol.1, by K.H.Davis,F.S.Berner,Edited by S.C. Bhatia (CBS Publishers, Bangalore,2004)
3. Industrial inorganic chemistry, Karl Heinz Buchel, Hans-Heinrich Moretto, Peter woditsch
4. Modern Electroplating , By M. Schlesinger and M. Paunovic (John Wiley and sons, Hoboken , New Jersey, 5th Edition 2010)
5. Insight into Specialty Inorganic Chemicals-David Thompson (The Royal Society of Chemistry,1995)-Chapter 15.
6. New Trends in Green Chemistry (2nd Edition)-V.K.Ahluwalia and M.Kidwai (Anamaya Publishers, 2007)

Section II: Inorganic Application in Medicine **(30 L)**

1. Overview (2L)

Introduction
Metal Ions in Disease
Use of chelating agents
Metalloproteins as Drug Targets
Matrix Metallopreteinases
Modulation of Cellular responses by Metal-Containing Drugs
Metal-Based Chemotherapeutic Drugs
Metal Complexes as Diagnostic Agents

2. Cisplatin-based Anticancer Agents (5L)
Introduction
Clinical Properties
Cisplatinvs carboplatin, Iproplatin
Determination of Platinum Drug Levels and Pharmakokinetics
Platinum Chemistry
Mechanism of Action
Structure-Specific Damage-Recognition Proteins
Mechanisms of Resistance to Cisplatin/Carboplatin
Circumvention of Tumor Resistance to Cisplatin
Development of New Platinum Drugs
Dose Intensification of Cisplatin/Carboplatin
Modulation of Platinum Resistance Mechanisms
Dinuclear and Trinuclear Platinum Complexes as Anticancer Agents
Biological Activity of Polynuclear Platinum Complexes. Summary and p53 status of Human Tumors Treatable by BBR3464
Biological Activity and p53 Status
Comparison with Other Clinical Cross-Linking Agents
Structure-Activity Relationships in Polynuclear Platinum Complexes
DNA Binding of Polynuclear Platinum Complexes
Cooperative Effects In the Solution Structures of Site-Specific (Pt,Pt) Interstrand Cross-Links

3. Transition Metal Complexes as Chemical Nucleases (4 L)
Interaction of Metal Complexes with DNA
Reactions of Metal Complexes with DNA
Nuclease activity of $Cu(phen)_2$ +

4. Biomedical Uses of Lithium (3L)
Chemistry of Lithium
Distribution of Lithium in the body and in Cells
Studies using Lithium isotopes
Biochemistry of Lithium

5. Bismuth in Medicine (3L)
The Chemistry of Bismuth
Properties of the element
Bi(III) Compounds
Bi(V) Compounds
Bismuth in Medicine
Helicobacter Pylori bacterium
Methods for the study of Bi
Bismuth Citrate Complexes
Bismuth Complexes with Biomolecules

Bismuth binding to oxygen-containing molecules
Bismuth Complexes with thiolate ligands
Bismuth(III) complexes with Metallothionine and Transferrin, Enzyme Inhibition

6. Gold Complexes with Anti-arthritic, anti-tumor and Anti-HIV activity (4L)
Introduction
Chrysotherapy,
History of Medicinal Uses
Gold Chemistry
Oxidation states
Gold(I) complexes
Gold(III) Complexes
Oxidation-Reduction Potentials
Gold Biochemistry and Pharmacology In-vivo metabolism and ligand displacement
Anti-tumor Activity
Anti-HIV activity

7. Vanadium Compounds as Possible Insulin Modifiers (3L)
Introduction
Characterization of Vanadium's Insulin-mimetic Effects
Sites of Action of Vanadium
Animal Studies and Human Trials
Toxicological Considerations
Improved Tissue Uptake with Metal Chelation

8. Radio metal-labeled agents (Non Technetium) for diagnostic imaging: (3L)
Introduction
Chemistry and biology of radio metals
Gamma scientigraphy and PET
Desirable properties of radio metals
Properties of radio metals- labeled imaging agents
Chemistry of radio metal- labeled imaging agents
Challenges in trivalent metal ion chemistry
Challenges in copper chemistry
Bifunctionalchelators for attaching radiometla to biomolecules.
Determining the optimal imaging agents foe specific diseases

9. Therapeutic Radiopharmaceuticals : (3L)
Introduction
Therapeutic radio nuclides
β- Particle emitting radionuclides
α- Particle emitting radionuclides
Low energy electron emitters

Therapeutic radiopharmaceuticals for routine medical use
^{131} I – sodium iodide
Intracavity and Intraarterial radiopharmaceuticals
Radiotherapeutic agents for bone cancer treatment
89 Sr-chloride
153 Sm- EDTMP
186 Re- HEDP and 117 Sn- DTPA
166 Ho- DOTMP
Site- directed therapeutic agent
64/67 Cu conjugates
186/188 Re labeled biomolecules

Books :

1.Uses of Inorganic Chemistry in Medicine Ed. Nicholas P.Farrell
2.Metal Complexes as drugs and chemotherapeutic agents
3.Metal Complexes as Enzyme inhibitors A.Y.Louie and Thomas Meade Chem.Rev., 1999, 99, 2711.

CHI-425: Advanced Techniques in Inorganic chemistry (5 credits; 60 Lectures)

1.Atomic X-Ray spectroscopy: (Ref. 3: p.343-371) (Ref.2 : p.340-392) (6L)

Fundamental principles , Instrument component, X-ray Fluorescence method, X-Ray absorption method, The electron microprobe, Electron spectroscopy for chemical analysis (ESCA) , Auger Emission spectroscopy (AES) , Problems

2. Atomic Emission Spectroscopy : (Ref. 2: p.260-284) (5L)

Introduction , Instrumentation , Typical applications , ICP atomic Fluorescence spectroscopy , Comparison of methods: ICP Vs AAS , Problems.

3. Raman spectroscopy (Ref. 1: p.533-549) (Ref.2.: p.321-336) (6 L)

Theory of Raman spectroscopy, Instrumentation, Sample handling and Illumination, structural analysis , polarization measurements, quantitative analysis , applications of Raman spectroscopy, other types of Raman spectroscopy, Comparison of Raman and Infrared spectroscopy, Problems

4. Mass Spectrometry: (Ref.2: p.465-507) (Ref. 1:p.606-664) (6L)

Molecular mass spectra , Sample flow in mass spectrometer, Inlet sample system , Ion sources , Mass spectrometers, Applications of molecular mass spectrometry , Quantitative application of mass spectrometry, ICP-MS , Secondary Ion Mass Spectrometry (SIMS) , Ion Microprobe Mass Analyzer (IMMA), Problems

5. Surface characterization by spectroscopy and microscopy (Ref.1: p.647-682) (6L)

Introduction to the study of surfaces , Spectroscopic surface methods ,, Electron spectroscopy, Ion Spectroscopic techniques , Surface photons spectroscopic methods , Electro- stimulated micro analysis methods , Scanning probe microscopies.

6. Particle size determination (Ref. 1: p. 1038-1051) (6L)

Introduction to particle size analysis , Low-angle Laser, light scattering , Dynamic light scattering , Photosedimentation.

7. Environmental sampling and analysis (Ref.3: ch.26,p.712) (6L)

Getting a meaningful sample , Air sample collection and analysis , Water sample collection analysis, Soil and sediment sampling, Sample preparation for trace organics , Contaminated land sites- what needs to be analyzed ? EPA method and Performance -based analysis.

8. Process instruments and Automated analysis (Ref. 2; p.786-826) (5L)

Introduction , Industrial process analyzers , Methods based on bulk properties, Infra red process analyzer , Oxygen analyzers , On-line Potentiometric analyzers , Chemical sensors , Process Gas Chromatography, Continuous on-line process control , Automatic chemical analyzers , Automatic elemental analyzers , Laboratory Robots , Problems.

9. Quality systems in Analytical measurements (Ref. 4.P. 45-65) (5L)

Introduction , Why is a quality system needed ? What is quality system? Benefits of a quality systems, Top-Down and Bottom –up, approaches to Quality, Quality standards and Accreditation , Valid analytical measurement programme , Proficiency testing, Validated methods , System suitability testing, Equipment Qualification, Quality Control of Instrument Performance.

10. Extended X-Ray Absorption Fine Structure (EXAFS) Analysis (Ref 5. Chap.9. p. 514-527,530-547) (5L)

EXAF theory- single scattering (SS) and multi scattering (MS) theory, Data analysis using GNXAS approach, GNXAS application to inorganic system, Implication of using GNXAS MS approach for study of biological system

11. LASER spectroscopy in Inorganic Complexes (Ref.5 Chap.6 p. 308-319 and 332-48) (4L)

Introduction, Fundamental principles , Laser sources and method , Tunable and single frequency Laser operation, Laser pulses –time and intensity dependent phenomena, Laser techniques such as Fluorescence and Excitation Line Narrowing (FLN and ELN) spectroscopy, Spectral hole burning , Photon echo measurement ,two photon and single molecule spectroscopy

Books:

1. Instrumental analysis – By Douglas A .Skoog, F. James Holler, Stanley R. Crouch (Publisher: cengageLearing India Pvt. Ltd . New Delhi , 2007)

2.Instrumental method of analysis (7^{th} edition) By- H.H. Willard , L.L. Merritt. Jr. J.A. Dean and F.A. Settle,Jr (Publisher: CBS Publishers and distributors Pvt .Ltd. (Copyright – wardsworth publishing copy USA .2000)).

3. Analyticalchemistry (6th edition) : By G.D. Christian (John Wiley and sons Pvt. Ltd. Singapore, 2009)

4. Analytical Instrumentation: Performance characteristics and Quality: By G.Currell (John Wiley and sons Pvt. Ltd. 2000) chapter .4

5. Inorganic Electronic Structure and Spectroscopy Volume 1, Methodology ; edited by Edward I. Soloman And A.B.P. Lever, (Wiley IntersciencePublication ,2013)

Practicals(Semester III)

CHI-328: Classical Inorganic Chemistry Practicals –I (4 credits, ~7.5 weeks)

CHI-329: Instrumental Inorganic Practicals-II (4 credits, ~7.5 weeks)

CHI-328: Classical Inorganic Chemistry Practicals –I (4 Credit ~7.5 weeks)

A + B = (3weeks) 12 days

A. Analysis: (3 weeks) 12 days

1. Stainless steel Alloy [e.g. iron, chromium and nickel from] 2d

2.Ilmenite Ore [e.g. acid-insoluble matter (combined oxides), iron and titanium from]2d

3.Analysis of Portland cement 2d

4.Pigment [e.g. chromium from Zinc chrome] 1d

5.Pharmaceutical products [e.g. magnesium from tablet of "Milk of magnesia", calcium from calcium-supplementary tablet, iron and zinc from iron- (and zinc)-supplementary capsule]1d

6.Consumer products [e.g. aluminium from alum] 1d

7.Ion exchange chromatography [separation and estimation of mixture of zinc (II) and magnesium (II)]1d

8.Purity & Percentage of Metal in Coordination Complexes. 2d

9. Organo metallic Compounds: Synthesis and characterization of Acetylferrocene 1d

B.InorganicPracticals (3 weeks) 12 days

Expt No. 1. Photometric Titrations

CuVs. EDTA

FeVs. EDTA using salicylic acid 2d

Expt No. 2. Photochemistry of ferrioxalate

a) Preparation

b) Photochemistry 2d

Expt.No. 3. &4 Kinetics by conductometry and spectrophotometry 3d

Preparation

Conductometry

Spectrophotometry

Expt No. 5. To study metal-DNA interaction spectrophotometrically 2d

Expt No.6. New Experiment related to Organometallic Chemistry or Homogenous Catalysis 2d

Expt No. 7. Flame photometry: determination of the percentage of sodium and calcium in the water sample 2d

Expt No. 8 Determination of phosphate in detergent by spectrophotometry 1d

Expt No. 9 Atomic absorption spectrophotometer (AAS): Demonstration and determination of amount of iron from tap water sample. 1d

Each experiment includes standardization of the reagents, calibration of the instrument with known reagents and analysis of an unknown

CHI-329: Instrumental Inorganic Practicals-II (4 credits, ~7.5 weeks)

A . Synthesis and Structural characterization of coordination compounds. (12 days)

1. Synthesis of coordination compounds: 3d

i) $M(acac)_2 \cdot xH_2O$ [where $M^{+2} = Mn^{+2}, Co^{+2}, Cu^{+2}$, x = 2,2,0 respectively]

$M(acac)_3$ [where $M^{+3} = Al^{3+} Mn^{+3}, Fe^{+3}$]

ii) trans-$[Co(en)_2Cl_2]Cl$ / cis-$[Co(en)_2Cl_2]Cl$

iii) $[Ni(en)_3]S_2O_3$ / Hg [$Co(SCN)_4$]

iv) [Fe (1, 2, 4-triazole $)_3$] $(ClO_4)_2$

Fe (DTC $)_3$

2. To determine paramagnetic susceptibility and magnetic moment of coordination compounds by Faraday method. (2d)

3. To determine paramagnetic susceptibility and magnetic moment of coordination compounds by Evan's ^{1}H nmr method. (1d)

4. To interpret IR spectra of acetylacetone and its complex. (1d)

i) To determine force constant of ⟩C=O bond.

ii) To determine bond lengths of ⟩C=O bond.

iii) To identify coordination site & type of coordination.

5. To interpret ESR spectrum of $Mn^{+2}(Oh)$ / $Co^{+2}(Oh)$ / $Cu^{+2}(D_{4h})$ etc. (1d)

To calculate magnetic parameters isotropic, anisotropic viz. g-factor, hyperfine coupling constant etc.

6. To interpret electronic spectra of coordination compounds.

i) To determine interelectronic repulsion parameter (B cm^{-1}) & crystal field parameter (10 Dq) using numerical fitting procedure.

ii) To calculate bonding parameters β_{35}. (2d)

7. To study cyclic voltammograms $K_3[Fe(CN)_6]$ (1d)

8. To interpret Mossbaur Spectra of iron salt (1d)

B. Solid State Materials: Preparation, characterization and activity: (12 days)

1. Preparation of solid-state materials: (a) NiO, (b) ZnO, (c) $ZnFe_2O_4$ or $NiFe_2O_4$, (d) Fe_3O_4, (e) $BaZrO_3$ or $SrZrO_3$ (2d)

2. To determine the interplanar spacing and lattice constant and crystallite size by using X-ray diffraction techniques (NiO, ZnO, Fe_3O_4, $ZnFe_2O_4$and Ni Fe_2O_4). (1d)

3. To determine the band gap of semiconducting materials (NiO / Fe_3O_4) by using direct current electrical conductivity measurement. (2d)

4. To find out the number of water molecules from coordination compounds/ hydrated metal salts by using thermogravimetric technique (TGA). (2d)

5. Heterogeneous catalysis.

(i) Photocatalytic degradation of dye using ZnO nanoparticles (2d)

a) time dependent

b) catalyst concentration

6. To determine the corrosion rate of metal strips (mild-steel / aluminium) in different conc. of acidic/ alkali medium. (2d)

8. To study the effect of 1, 10 phenanthroline on corrosion inhibition of mild-steel in H_2SO_4(1d)

Each experiment includes standardization of the reagents, calibration of the instrument with known reagents and analysis of an unknown

Practicals (Semester IV)

CHI-428: Project Work (7 credits, 13.5 weeks)