SAVITRIBAI PHULE PUNE UNIVERSITY, PUNE

SYLLABUS FOR

University Department

Master of Science
In
Inorganic Chemistry

PART-I and II

(Semester I, II, III and IV-choice based Credit system**)**

w.e.f. July 2018

Total Number of Credits: 80

Semester I		
Subject Code	**Subject Title**	**Number of Credits**
IC 120	Symmetry, Group Theory and Spectroscopy	4
OC 130	Reaction Mechanisms in Organic Chemistry	4
PC 140	Kinetics and Thermodynamics in Chemistry	4
Elective Courses (any one)		
IC 125	Physical Methods in Inorganic Chemistry and Main Group Chemistry	4
OC 135	Stereochemistry of Organic Reactions	4
PC 145	Chemical Mathematics and Elements of Computer Programming	4
Practicals for First Year		
IC 128	Experiments in Inorganic Chemistry	4
OC 138	Experiments in Organic Chemistry	4
PC 148	Experiments in Physical Chemistry	4
Semester II		
IC 220	Coordination and Bioinorganic Chemistry	4
OC 230	Synthetic Organic Chemistry and Spectroscopy	4
PC 240	Chemical Bonding and Molecular Spectroscopy	4
Total Number of Credits: 40		

Semester III		
Subject Code	**Subject Title**	**Number of Credits**
IC 320	Physical Methods in Coordination- and Bio-inorganic Chemistry	4
IC 321	Organometallic Chemistry and Homogeneous Catalysis	4
Elective Courses		
IC 325	Frontiers in Material Science and Analytical Techniques for Solids	4

IC 326	Inorganic Reaction Mechanism and Photochemistry	4
Practicals for Second Year		
IC 328	Experiments in Inorganic Chemistry I	4
IC 329	Experiments in Inorganic Chemistry II	4
Semester IV		
IC 420	Inorganic Polymers, Clusters and Heterogeneous Catalysis	4
IC 421	Solid State Chemistry of Inorganic Materials	4
Elective Courses (any two)		
IC 425	Industrial Inorganic Chemicals and Medicine Chemistry	4
IC 426	Advanced Techniques in Inorganic Chemistry	4
IC 427	Research Project	4
Total Number of Credits: 40		

UGC recommended courses (Additional 10 credits)		
Subject Code	**Subject Title**	**Number of Credits**
	Cyber security/Information security	4
	Skill based credits	4
	Human rights education	2

Courses which can be opted by students from outside departments:

Sub. Code	**Subject Title**	**Number of Credits**
Elective courses		
	Semester- III	
IC 325	Frontiers in Material Science and Analytical Techniques for Solids	4
	Semester- IV	
IC 425	Industrial Inorganic Chemicals and Medicine Chemistry	4
IC 426	Advanced Techniques in Inorganic Chemistry	4

SEMESTER-I

IC 120: Symmetry, Group Theory and Spectroscopy (4Credits, 60L)

1. Definitions and theorems of group theory, subgroups, classes. **(4L)**

2. Molecular symmetry and symmetry groups - symmetry elements and operations. Symmetry planes reflections, inversion centre, proper / improper axes and rotations, products of symmetry operations , symmetry point groups ,classes of symmetry operations, classification of molecular point groups. **(10L)**

3. Representations of groups. Great orthogonality theorem, character tables, properties of characters of representations. **(8L)**

4. Group theory and quantum mechanics. Wave function as bases for irreducible presentation. **(2L)**

5. Symmetry Adapted Linear Combinations - (SALC) - projection operators and their use to construct SALC. **(6L)**

6. Molecular Orbital Theory.
Transformation properties of atomic orbitals, MO's for Sigma bonding in ABn molecules, tetrahedral AB_4 case, Hybrid orbital's, MO's for pi bonding in ABn molecules. **(10L)**

7. Application of group theory to infrared spectroscopy (Ref.-2, Chapter-8)
Introduction, selection rules, polyatomic molecules, possible vibration in a linear molecule, bending modes, symmetry of vibrations and their IR activity, Group vibration concept and its limitations, IR spectra related to symmetry of some compounds, IR spectra of complex compounds. **(10L)**

8. Raman spectroscopy:
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 (Ref. 7: p.533-549) (Ref.8: p.321-336) **(10L)**

Books

1. Chemical applications and group theory F.A. Cotton, 3rd edition, John Wiley & Sons Asia Pvt. Ltd. (1999).
2. Group theory and its chemical applications: P.K Bhattacharya, 2nd edn, Himalaya pub. India,(1989).
3. Molecular symmetry and group theory -A. Vincent.
4. Symmetry in Chemistry: H.H. Jaffe' and M. Orchin, Dover Publications Inc, New York,(2002).
5. Symmetry in Inorganic Chemistry: J.P Fackler.
6. Principles of Materials Science and Engineering: William F. Smith (1980) (Chapter 3)

7. Instrumental analysis – By Douglas A .Skoog, F. James Holler, Stanley R. Crouch (Publisher: Cengage Learing India Pvt. Ltd . New Delhi , 2007)
8. Instrumental method of analysis (7th 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 – Wordsworth publishing copy USA .2000).

OC 130: Stereochemistry and Reaction Mechanism **(4 Credits, 60L)**

Aromatic Electrophilic substitution reactions **(15)**

Arenium ion mechanism, orientation and reactivity, energy profile diagram, calculation of partial rate factor, the ortho/ para ratio, Ipso substitution, Orientation in other ring systems such as Naphthalene, Anthracene, six and five membered heterocycles, Diazonium coupling, Vilsmeier reaction, Gattermann–Koch reaction etc. The $ArSN^1$, benzyne and SNR1, mechanisms, reactivity effect of substrate structure, leaving group and attacking nucleophile.

Kineticandnon-kineticmethods (**7**)

Hammond Postulate, Curtin-Hammett Principle, Microscopic Reversibility, Kinetic/Thermodynamic Control, First, Second and Pseudo-First Order Kinetics, trapping of intermediate(s), competition experiments, testing proposed/common intermediate, isolation and identification, characterization using spectral methods of product and intermediate, Cross-over experiments, Structure variation methods, Stereochemical analysis, Isotope labeling, Techniques to study radicals, Transient spectroscopy.

Hammett equation: (**8**)

Substituent constant, reaction constant, +ve, -ve rho values, reaction with small -ve rho values, interpretation of mechanism using rho values, non-linear Hammett plots, kinetic isotopic effect, entropy of activation.

Molecular rearrangement and reaction intermediate (**15**)

Structure, generation and stability of carbenes, nitrenes, carbocations and carbanions intermediates. Rearrangement reactions *viz*. Beckmann, Curtius, Hofmann, Lossen, Favorskii, Baeyer-Villiger, Wolff, Claisen, Pummerer, Wagner-Meerwin, Stevens, Dienone-Phenol, Sommelet-Hauser, Benzilic acid, Benzidine, Cope, Fries and Schmidt reaction.

Basic Concept of Stereochemistry of Organic Compounds **(15)**

Origin of Stereochemistry, Optical activity, Chirality and molecular symmetry, axial and central chirality. Projection formulae, Configuration (D/L, d/l, R/S, E/Z configuration in C, N, S, P containing compounds), Allenes, biphenyls and spiranes nomenclature and enantiomerism. Optical activity in biphenyls, spiranes, allenes and helical structures. Enantiomeric and distereomeric relationship, Isomerism in molecules with more than one chiral center, Pseudo-asymmetry, Prochirality. Enantomeric excess.

Books/References:

1. Organic Chemistry by J. Clayden, N. Greeves, S. Warren and P. Wothers (Oxford)
2. Advanced Organic Chemistry by J. March 6^{th} Edition
3. Advance Organic Chemistry (part A and B) by A. Carey and R. J. Sundberg
4. Stereochemistry of carbon compound by E. L. Eliel

5. Stereochemistry of organic compound by Nasipuri
6. The Hammett equation, C. D. Johnson, Cambridge University Press (1973)

PC 140: Kinetics and Thermodynamics in Chemistry (4 credits, 60L)
Chemical Kinetics: (2 credits, 30L)

1. Recapitulation:
   Rate of Reaction, empirical rate law, rate constants, order, molecularity, half-life and life time of reaction. Zeroth first and second, third and half-integral order reactions, methods to determine order of the reactions and temperature dependence of reaction rates (5L)
2. Complex reactions:
   Rate laws for complex reactions, parallel reaction with example of nuclear reactions and fluorescence decay, opposing reactions, rate constants by temperature jump method, consecutive reactions, rate determining step and steady state approximation (7L)
3. Approximate methods to solve complex reactions:
   Steady state and pre-equlibrium approximations, Lindemann mechanism for the unimolecular reaction. Enzyme catalysis – Michaelis Menton Mechanism, Lineweaver and Eadie plots, Chain reactions: free radical polymerization, oscillating reactions (8L)
4. Method of studying fast reactions:
   Flash photolysis, stop flow technique, pump and probe methods (3L)
5. Molecular reaction dynamics:
   Collision theory for bi-molecular reactions (derivation expected), steric factor, Transition state theory, Eyring equation (derivation expected)-thermodynamic aspects –entropy. – enthalpy and free energy of activation, effect of dielectric constant on the ionic reactions, primary and secondary salt effect, effect of pressure on the reaction rates. Linear free energy relationships (7L)

Text Books:

1. Atkins' Physical Chemistry, Peter Atkins and Julio e Paula ninth edition Oxford University Press 2011.
2. Physical Chemistry, D.A. McQuarrie, Viva Book private limited, 1998.
3. Chemical Kinetics, K. J Laidler, Third edition, Pearson Education Inc., 1987.

Thermodynamics (2 Credits, 30L)

1. Zeroth, first and second law of thermodynamics, dependence of enthalpy, free energy and entropy on pressure and temperature, free energy change and equilibrium constant, partial molar quantities–Maxwells equations and their applications, Third law of thermodynamics and its applications, residual entropy (13L)
2. Thermodynamics of Real Gases
   Concept of activity, choice of standard states, Methods of determining activity coefficient and activity coefficient, variation of activity and activity coefficient of a gas with pressure and temperature, concept of fugacity, fugacity of a gas in mixture of real gases (7L)
3. Statistical Thermodynamics
   Boltzmann distribution law, partition functions and ensembles, calculation of translational, rotational and vibrational partition functions, statistical thermodynamics

and Third Law of Thermodynamics, internal energy, heat capacity, entropy, free energy, equilibrium constants (10L)

Text/Reference Books

1. Physical Chemistry, P. W. Atkins, Sixth Edition, Oxford University Press, Oxford (1998).
2. Physical Chemistry, T. Engel and P. J. Reid, Benjamin-Cummings (2005).
3. Physical Chemistry, G. M. Barrow, Fifth Edition, Tata McGraw Hill, New Delhi.

Elective Courses (any one)

IC 125: Physical Methods in Inorganic Chemistry and Main Group Chemistry (4Credits, 60L)

(a) Main Group elements: (30 Lectures)

1. Hydrogen & its compounds (2L)
Hydrides, classification, e- deficient, e- precise & e- rich hydrides PH3,SbH3,AsH3, Selenides, Tellurides.

2. Alkali & alkaline earth metals (4L)
Solutions in non-aqueous Media. Application of crown ethers in extraction of alkali & alkaline earth metals.

3. Organometallic compounds of Li, Mg, Be, Ca, Na (2L)
Synthesis, properties, uses & structures.

4. Boron group (4L)
Boron Hydrides, preparation, structure & bonding with reference to LUMO, HOMO, interconversion of lower & higher boranes, Metalloboranes, Carboranes.

5. Carbon group (4L)
Allotropes of Carbon, C60 and compounds (fullerenes), Intercalation compounds of Graphite, Carbon nanotubes, synthesis, properties, structure-single walled, multiwalled, applications, classification of organometallic compounds. Organometallic compounds of B, Si, Sn,Pb, Ga, As, Sb, Bi. Structures, Synthesis, Reactions

6. Nitrogen group (4L)
Nitrogen activation, Boron nitride, Oxidation states of nitrogen & their nterconversion PN & SN compounds NOx & their redox chemistry

7. Oxygen group (4L)
Metal selenides & tellurides, oxyacids & oxoanions of S & N, Ring, Cage and Cluster compounds of p-block elements. Silicates, including Zeolites

8. Halogen group (4L)
Interhalogens, Pseudohalogen, synthesis, properties & applications, structure, oxyacids & oxoanions of Hallogens Bonding.

9. Noble gases (2L)
Synthesis, properties, uses, structure & bonding with respect to VSEPR.

(b) Physical Methods in Inorganic Chemistry (30 Lectures)

1. **Crystal Structure and Crystal geometry (08)**

Space Lattice and basic unit cells, Crystal systems and Bravais Lattices, Classification of space lattice by crystal systems and their structures, the relation between interatomic distance (d) and atomic radius(R) of cubic unit cells. The Atomic Packing factor of BCC, FCC and HCP unit cell and their examples, Atomic positions in cubic unit cells with origin at eight corners of the cube, directions in Cubic Unit Cells, Direction Indices in cubic unit cells, Miller indices for crystallographic planes in Cubic unit cells, Crystallographic planes in Hexagonal unit cell, Miller-Bravais indices. Volume, planar and linear density calculations of cubic unit cells, application of Miller indices in solving crystal structures, problems of all the topics.

2. **NMR of Inorganic Compounds (10)**

Concept of nuclear spin and resonance, fundamentals of coupling (homonuclear heteronuclear) and decoupling, coupling constants. Predicting Intensity of NMR lines by binomial, trinomial, tetranomial etc Pascal triangles Examples of ^{11}B and ^{10}B NMR, ^{1}H and ^{11}B NMR spectra of of BH_4^-, $Me_4{}^{11}B_2H_2$, $Me_2B(\mu\text{-}H)_2BH_2$, second order coupling in diborane, Effect of natural abundance. Structure elucidation by ^{19}F and ^{31}P NMR spectroscopy. Examples: ^{19}F NMR spectra of interhalogen compounds, ^{19}F and ^{31}P NMR to deduce structures of PF_3R_2 type compounds, ^{31}P NMR of Wilkinson catalyst, geometrical isomers of platinum compounds, *trans effect* and *meridonial*, *facial* isomers of rhodium compounds. General trends in chemical shifts, factors influencing chemical shift-geometry, electronegativity, charge and oxidation state, coordination number, effect of ligands, coordination effect on transition metal. General trends in coupling constant, factors influencing coupling constant- gyromagnetic ratio, periodicity, ‘s’ character in the bond, hybridization, coordination number, electronegativity, trans effect, inter bond angles lone pairs and oxidation state.

3. Mössbauer spectroscopy(12)

Basic principles of ^{57}Fe Mössbauer spectroscopy, instrumentation, spectral parameters

a) Mössbauer Parameters- Isomer Shifts, quadrupole splitting, Magnetic hyperfine interaction.

b) Application of Mössbauer spectroscopy with respect to

i) Oxidation states of metal ion in compounds

ii) Structural elucidation

iii) Covalent and ionic compounds

iv) High spin low spin behavior

v) Magnetically ordered compounds

Books:

1. Advanced Inorganic Chemistry: F. A. Cotton, G. Wilkinson,C. A. Murollo, M. Bochmann, 6th edn. (2003).
2. Inorganic Chemistry: D. F. Shriver and P.W. Atkins, 4th edn. Oxford (2003).
3. Concise inorganic Chemistry, J.D.Lee 4Th edition (Chapman and Hall)
4. Physical Methods in Chemistry, R. S. Drago, Saunders, Harcourt Brac Javanovich College Publishers, (1992).
5. NMR spectroscopy in Inorganic Chemistry, J. A. Iggo, Oxford University press (2001).
6. Mössbauer Spectroscopy and Transition Metal Chemistry, P. Gütlich,R. Link, A. Trautwien, Springer-Verlag (1978).
7. Mössbauer Spectroscopy, N.N. Greenwood, T.C. Gibb, Chapman and Hall Ltd. (1971).
8. Instrumental method of analysis (7th 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).

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6. The Hammett equation – C. D. Johnson, Cambridge University Press (1973)

PC 145: Chemical Mathematics and Elements of Computer Programming (4 Credits, 60L)

Chemical Mathematics (3 Credits, 45 L)

1. Functions, differential and integral calculus, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, applications in chemistry, exactand inexact differential, Taylor and McLaurin series, curve sketching, partial differentiation, rules of integration, definite and indefinite integrals, integral involving exponential and Gaussian functions (27L)
2. Differential equations
   Separation of variables, homogeneous, exact, linear equations, equations of second order, series solution method. (6L)
3. Probability
   Permutations, combinations and theory of probability (4L)
4. Vectors, matrices and determinants
   Vectors, dot, cross and triple products, introduction to matrix algebra, addition and multiplication of matrices, inverse, adjoint and transpose of matrices, unit and diagonal matrices, (4L)

5. Special functions, Gamma functions, hermite polynomials, Legendre polynomials, Laguerre functions – definitions and recursion relation (no proof required) (4L)

Elements of Computer Programming (1 credit, 15L)

Hardware and software, binary and decimal numbers, constants and variables, assignment statement, flow chart and their use, IF and GO TO statements, Do loops. Input, output and format statements, Subroutines, function subprograms, Algorithms, Introduction to programming languages (15L)

Text Books

1. The Chemical Maths Book, E. Steiner, Oxford University Press (1996).
2. Maths for Chemists, Volumes 1 and 2, Martin C. R. Cockett and Graham Doggett, Royal Society of Chemistry , Cambridge (2003).
3. Computers and Common Sense *R. Hunt and Shelley*, Prentice Hall, New Delhi (1998)
4. Computer Programming in Fortran-90 V. *Rajaraman*, Prentice Hall, New Delhi (1990)
5. Computer and Chemistry: introduction to programming and numerical methods *T. R. Dickson*, Freeman (1968)
6. Computer programs for chemistry *D. F. Detar* W. A. Benjamin Inc, New York Vol. 1-3 (1968-69)
7 Mathematical Preparation for Physical Chemistry, F. Daniels, McGraw Hill (1972).

Practicals for First Year

IC 128: Experiments in Inorganic Chemistry (4 Credits, 9 weeks)

1**.** Ore Analysis: At least two of the following:
a. Determination of silica and manganese in pyrolusite .
b. Determination of copper and iron from chalcopyrite.
c. Determination of silica and iron from hematite

2. Alloy analysis (At least two of the following)
a. Determination of tin & lead from solder.
b. Determination of iron & Chromium from mild steel.
c. Determination of copper and nickel from cupronickel.

3. Inorganic Synthesis and purity determination (any five)
a. Cis-trans potassium di-aquo di-oxalato chromate (III)
b. Chloro penta-ammino cobalt (III) chloride
c. Nitro penta-ammino cobalt (III) chloride
d. Nitrito penta-ammino cobalt (III) chloride
e. Bis,2-4 pentanedionato cobalt (II) and cobalt (III)
f. Potassium tri-oxalato aluminate

4. Ion-exchange chromatography
Separation of mixture of Zn(II) and Mg(II) using Ammberlite IRA 400 anion exchanger and quantitative estimation of separated ions Zn(II) and Mg(II)

(a) Chelation in Nickel complexes: Preparation of Ni (II) ethylenediamine complexes and studying their absorption spectra.

(b) Solution state preparation of [Ni(en)3]S2O3, [Ni(H2O)6]Cl2, [Ni(NH3)6]Cl2. Record the absorption spectra in solution of all three complexes and analyze it. Arrange the ligands according to their increasing strength depending on your observation

5. Instrumental methods of analysis.

a. Colorimetry.

1. Simultaneous determination of Cr & Mn.
2. Determination of Keq of M-L Systems such as ,
   Fe (III) - salicylic acid, Fe (III)-Sulphosalicylic acid
   Fe (III) - b -resorcilic acid by Job's & Mole- ratio method.

b. Determination of iron by solvent extraction technique in a mixture of Fe3+ + Al 3+ & Fe3+ + Ni2+ using 8- hydroxyquinoline reagent.

c. Study of aquation of [Fe(o-phen)3] in acid solution by spectrophotometry.

d. Conductometry (Ref.- 5)

i.Verification of Debye Hückle theory of ionic conductance for strong electrolytes KCl,BaCl2.K2SO4, K3[Fe(CN)6]

ii.Structural determination of metal complexes by conductometric measurement

iii. To study complex formation between Fe(III) with sulfosalicylic acid by conductometry

e New Experiments : (any one)

i. Data analysis, error analysis, least squares method. Plot of Born Maeyer to determine for 1:1 type molecule to determine internuclear separation. Characterization of metal ligand bonding using IR spectroscopy.

ii. Computer Applications: (1) Electronic structure, vibrational characteristics and charge distributions in first row transition metal complexes. (2) Visualizing frontier MO's.

iii. Analysis of Electronic spectra of transition metal complexes at least for one system (dn Oh or Td) and calculation of Crystal Field parameters, inter electronic repulsion parameter and bonding parameter.

References:

1. Textbook of Quantitative Analysis, A. I. Vogel. 4th edn (1992).
2. Inorganic Electronic spectroscopy: A. B. P. Lever, 2nd edn Elsevier Science Publishers, New York, (1984).
3. Inorganic Synthesis (Vol. Series)
4. Practical Manual made By Department of Chemistry, University of Pune
5. Experiments in Chemistry, D.V. Jahagirdhar, Himalaya Publishing House

OC-138: Organic Chemistry practical (Departmental Course) (**4 Credits**)

1. Practical techniques: Crystallization, fractional crystallization, distillation, fractional distillation, sublimation, thin layer chromatography and column chromatography.
2. Derivatives: Acetyl, 2,4-DNP, anilide, amide, aryloxy acetic acid etc.
3. At least two Oxidation and Reduction reactions

4. Single stage preparations (6 preparations) based on regio-selective and chemo selective principals
5. Two stage preparations (6 preparations)

Note-i) Preparations preferred to be club with various technics and ii) Preparation preferred to be on the aromatic substitution, Nucleophilic substitution, Free radical substitution, Addition, Elimination Condensation, Rearrangements, Oxidation, Reduction etc.

PC 148: Experiments in Physical Chemistry (4 Credits)

Conductometry:

1. Hydrolysis of NH4Cl or H3COONa or aniline hydrochloride
2. Solubility of a sparingly soluble salt.
3. Hydrolysis of ethyl acetate by NaOH.
4. Determination of DG, DH, and DS of Silver Benzoate by conductometry.

Potentiometry:

1. Stability constant of a complex ion.
2. Solubility of a sparingly soluble salt.
3. Determination of dissociation constant of acetic acid.
4. Estimation of halide in mixture.
5. pH metry.
6. Hydrolysis of aniline hydrochloride.
7. Determination of the acid and base dissociation constants of an amino acid and hence the isoelectric point of the acid.
8. To determine the amount of aspirin in the given tablet.

Colorimetry:

1. Analysis of a binary mixture.
2. Copper EDTA photometric titration.
3. Determination of stability constant of ferricsalicylate complex by colorimetric measurements

Radioactivity:

1. Half-life of a radioactive nuclide.
2. Determination of Emax of beta radiation and absorption coefficients in Al.
3. Counting errors.

Chemical kinetics:

1. Kinetic decomposition of diacetone alcohol by dilatometry.
2. Determination of an order of a reaction.
3. Bronsted primary salt effect.
4. Kinetics of the reduction of methylene blue by ascorbic acid.

Non-Instrumental:

1. Freundlich and Langmuir isotherms for adsorption of acetic acid on active charcoal.
2. Molecular weight by steam distillation.
3. Glycerol radius by viscosity.
4. Partial Molar volume (Pycnometry)
5. Determine the viscosities of mixtures of different compositions of liquids and find the composition of a given mixture.

Computer applications:

1. Least square fitting of experimental data.

Each candidate should perform a minimum of 20 experiments with at least two experiments from each technique.

Text Books

1. Findlay's Practical Physical Chemistry, B. P. Levitt and J.A. Kitchener 9th Edition, Longmans, London (1972).
2. Experiments in Physical Chemistry by J. M. Newcombe, R. J. Denaro, A. R. Rickett, R.M.W Wilson, Pergamon (1962).
3. Senior Practical Physical Chemistry, 5th Edition, B. D. Khosla, V. S. Garg and A. Khosla, R. Chand (1987).

SEMESTER II

IC 220: Coordination & Bioinorganic Chemistry (4Credits, 60L)

(a) Coordination Chemistry

1. Concept & Scope of ligand Fields. **(1L)**

2. Energy levels of transition metal ions, Free ion terms, spin –orbit coupling. **(7L)**

3. Effect of ligand fields on energy levels of transition metal ions, weak cubic ligand field effect on Russell-Saunders terms, strong field effect, correlation diagrams, Tanabe-Sugano diagrams, Spin-pairing energies. **(8L)**

4. Electronic spectra of complexes, band intensities, band energies, band width & shapes, spectra of 1st, 2nd & 3rd row ion and rare earth ion complexes, spectrochemical & Nephelauxetic series, charge transfer & luminescence spectra, calculations of Dq, B, ı parameters. **(8L)**

5. Magnetic properties of complexes, paramagnetism,1st & 2nd ordered Zeeman effect, quenching of orbital angular momentum by Ligand fields, Magnetic properties of A,E,T ground terms in complexes, spin free–spin paired equilibria. **(6L)**

(b) Bioinorganic Chemistry

6. Overviews of Bioinorganic Chemistry. **(2L)**

7. Principles of coordination Chemistry related to Bioinorganic–Proteins, nucleic acids and other metal binding biomolecules **(6L)**

8. Choice, uptake and assembly of metal containing units in Biology **(6L)**

9. Control and utilization of metal ion concentration in cells. **(6L)**

10. Metal ion folding and cross –linking of biomolecules. **(6L)**

11. Binding of metal ions and complexes to biomolecular active Centers **(4L)**

Books:

1. Ligand field theory & its application: B.N.Figgis & M.A.Hitchman Wiely VCH publ. (2000), Chapters 5, 6, 8,9,11.

2. Principles of Bioinorganic Chemistry: S.J.Lippard & J.M Berg, University science books, Mill Valley, California (1994), Chapters- 1,2,3,5,6,7,8.

3. Inorganic Chemistry: D. F. Shriver & P. W. Atkins, Oxford (1999).

4. Inorganic Electronic spectroscopy: A. B. P. Lever, 2nd edn Elsevier Science Publishers, New York, (1984).

5. Biological Chemistry of the Elements: R. J. P. Williams & F. R. De Salvia, Oxford University Press-(1991).

6. Bioinorganic Chemistry: Inorganic elements in the Chemistry of life: An introduction and guide:W. Kaim, B. Schwederski,VCH,(1991).

OC 230 – Synthetic Organic chemistry and Spectroscopy (4 credits, 60L)

Oxidation and Reduction: (**12**)

Oxidation Reactions: CrO_3 (Jones reagent) PDC, PCC, $KMnO_4$, MnO_2, Swern Oxidation, SeO_2, $Pb(OAc)_4$, Pd/C, OsO_4, m-CPBA, O_3, $NaIO_4$, HIO_4, R_3SiH, Bu_3SnH, Reaction of NBS. Reduction viz. Wilkinson's catalyst, metal hydrides, $NaCNBH_3$, NH_2NH_2, DIBAL, Zn, etc. Stereochemistry involved in hydrogenation, hydroboration, B.V. oxidation, $KMnO_4$, OsO_4, $Pb(OAc)_4$, oxymercuration, Wilkinson's catalyst, O_3, $NaIO_4$, HIO_4 etc.

Ylids:Phosphours, sulphur and nitrogen, synthesis and applications (**5**)

Organo-metallic chemistry: (**10**)

Li, Zn, Cu, Mg, Al, Si etc., Hydroboration and synthesis of borane reagents and its use in oxidation and protonation.

Spectroscopy: (**18**)

Basics of UV, IR and NMR. Instrumentation and recording of spectra of UV, IR and NMR, Elementary ideas of NMR, integration, chemical shifts etc. Factors affecting chemical shifts, Coupling (First order, analysis), Problems based on UV, IR and NMR.

Heterocyclic Chemistry: (**15**)

Structure, reactivity, synthesis and reactions of pyrrole, furan, thiophene, pyridine, indole, benzofuran, quinolone and isoquinoline.

Books/References:

1. Carey and Sundberg. (Ed. IV), Part B – Adv. Organic Chemistry.

2. H.O. House, Synthetic Organic Chemistry.
3. Norman R.O.C. Organic Chemistry.
4. Advanced Organic Chemistry by J. March 6thEdition
5. Silversteine and Basser, Spectrometric Identification of Organic Compounds.
6. P.S. Kalsi, Organic Spectroscopy.
7. J. Bellamy, Infrared spectra of Complex molecules.
8. I Fleming, Organic Spectroscopy.
9. J. Clayden, N.Greeves et. al Organic Chemistry
10. Pavia Spectroscopy of Organic Compounds
11. Heterocyclic Chemistry – J. A. Joule, K. Mills and G. F. Smith

PC 240: Chemical Bonding and Molecular Spectroscopy (4 Credits, 60 L)
Chemical Bonding (2 Credits, 32 L)

1. Recapitulation, quantization, Postulates of Quantum mechanics, Schrödinger equation, particle in a box, particle in 3-D box, degeneracy, hydrogen-like atoms (no derivation), atomic orbitals. (12 L)
2. Variational method, many electron atoms, orbital angular momentum, electron spin, wave functions of many electron atoms, Pauli exclusion principle, spin-orbit interaction, fine structure, vector atom model, spectral terms. (5 L)
3. Molecular orbital theory, Born-Oppenheimer approximation, H2 molecule, homo and hetero-nuclear diatomic molecules, MO diagrams of simple triatomic molecules. (5 L)
4. Valence bond theory of simple molecules, quantitative treatment of hydrogen molecule and related systems, hybridization, comparison of VBT and MOT. (4 L)
5. Hückel theory of conjugated hydrocarbons, Electron densities, Bond orders and free valence indices, Illustrations (6 L)

Text Books

1. Quantum Chemistry, I. Levine, 5th Edition, Prentice Hall (1999).

Reference Books

1. Valence, C. A. Coulson, ELBS (1974).
2. Introduction to Quantum Mechanics- with Applications to Quantum Chemistry, L. Pauling and E. B. Wilson, Dover Publishers (1999).
3. Orbitals in Chemistry, V. Gil, Cambridge University Press (2000).

Molecular Spectroscopy (2 Credits, 28 L)

1. Recapitulation, regions of electromagnetic spectrum, width and intensity of spectral lines. (2 L)
2. Rotational spectra: classification of molecules based on the moment of inertia, Schrodinger equation of rigid rotor, diatomic molecules, effect of isotopic substitution, centrifugal distortion, linear triatomic molecules, symmetric top molecules, stark effect. (5 L)
3. Infrared spectra: quantum mechanical harmonic oscillator, diatomic molecule, Morse potential, overtone and hot bands, polyatomic molecules, skeletal and normal vibrations (6 L)

4. Vibrational rotational spectra, fine structure in diatomic molecules, break down of the Born-Oppenheimer approximation, effect due to nuclear spin, parallel and perpendicular vibrations. (4 L)
5. Raman Spectra: classical and quantum theory of Raman effect, stokes and antistokes lines, polarizability ellipsoid, rotational Raman spectra, selection rule, vibrational raman spectra, rule of mutual exclusion, elucidating structure from the combined infrared and Raman spectra, rule of mutual exclusion (6 L)
6. Electronic spectra: Born-Oppenheimer approximation, molecular progression, term symbols, Franck-Condon principle, dissociation energies, oscillator strength, rotational fine structure, fortrat parabola, predissociation, photoelectron spectroscopy (5 L)

Text Books

1. Fundamentals of Molecular Spectroscopy, C. M. Banwell and E. McCash, Tata McGraw Hill, 4th Edition (1994).
2. Molecular Spectroscopy, J. Machale, Prentice Hall, NJ, USA (1999).
3. Vibrating Molecules, P. Gans, Chapman and Hall, UK (1971).

SEMESTER III

IC 320: Physical methods of coordination compounds and Bio-inorganic chemistry (4Credits, 60L)

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 d2 and p2, transition metal ions.
Derivation of Van Vleck's expression and □S+O formula, Quantization of orbital contribution in d1 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:
(a) Structural determination of Inorganic complexes.
(b) Applications metalloproteins, Fe, Cu.

3. Nuclear Quadrupole Resonance (NQR) **(3)**
(a) Principle selection rule for NQR
(b) Factos for splitting of quadruple energy levels in NQR
(c) 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:

1. Magnetism and Transition Metal Complexes, F. E. Mabbs and D. J. Machin (Chapman and Hall) London (1973).
2. Introduction to Magnetochemistry, A. Earnshaw, Academic Press, (1968).
3. Elements of Magnetochemistry, R. L. Dutta and A. Syamal, Affiliated East/West Press Pvt. Ltd. 2007.
4. Physical Methods in Chemistry, R. S. Drago (2nd Edition) (1977).
5. 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 **(2L)**
Structural Information
Metal Activity, Specificity & Selectivity
Biochemical Evolution of Metals in Biological System

(2) Biological Chemistry of Iron **(4L)**
Transport of Iron
Hemoglobin & Myoglobin (including their model compounds)
Cytochromes
Ribonucleotidereductase

(3) Biochemistry of Cobalt **(3L)**
B12 Coenzymes and Model compounds
Actions of Cobalmins&Cobinamides
Adenosylcobalmin as a Coenzyme
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
Molybdenum 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)**
Carboxypeptidase and Carbonic anhydrase enzymes
Alcohol dehydrogenase

(8) Biological Chemistry of Manganese **(4L)**
Photosystem II
Water oxidation center and S4 cycle
Catalases and peroxidases

Books :

1. Bioinorganic Chemistry : A Short Course –Rosette M. Roat-Malone, Wiley Interscience, 2002.
2. Biological Inorganic Chemistry –An Introduction, Robert Crichton, Elsevier Science, 2007
3. 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.
4. Bioinorganic Chemistry by Nils Metzler-Nolte

IC 321: Organometallic Compounds and Homogeneous Catalysis (4Credits, 60L)

Section I: Organometallic Chemistry (30 lectures)

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

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

3. □-organyls : Synthesis, bonding, Properties and applications of Alkyls, aryls, alkenyls, acyl, alkynyls **(5)**

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

5. □-complexes: Alkenes, d—and polyenes **(2)**

6. □n-CnRn carbocyclic polyenes : Synthesis, bonding, Properties and applications of allyls□3-C3R5 , pentadienyls□5-C5R7, cyclopropenyls□3-C3R3, cyclobutadienes□4-C4R4 cyclopentadienyls□5-C5R5, arenas □6-C6R6, cycloheptatrienyls□7-C7R7, cyclooctatetraenes. **(6)**

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.
4.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 , Asymmetricpalladium catalyst, Rhodium Catalysts for asymmetric ketone reduction .
10. Asymmetric Catalysis: General features of chiral ligandsand complexes; Mechanisms and Catalytic cycles in hydrogenation, isomerization, epoxidation and catalytic reactions of C-C bond formation

Books :

1. Homogeneous Catalysis: The Applications and Chemistry of Catalysis by Soluble Transition Metal Complexes, G.W. Parshall and S.D. Ittel, Wiley, New York 1992
2. Applied Homogeneous Catalysis with Organometallic Compounds, Vols. 1 & 2, edited by B. Cornils and W.A. Herrmann, VCH, Weinheim, New York, 1996
3. Homogeneous Catalysis: Mechanisms and Industrial Applications, S. Bhaduri and D. Mukesh, Wiley, New York, 2000
4. Homogeneous Catalysis: Understanding the Art, P.W.N.M. van Leeuwen, Kluwer Academic Publishers, 2003

IC 325: Frontiers in Material Science and Analytical Techniques for Solids (4Credits, 60L)

Section I Frontier's in material science (30 lectures)

1. The Structure of solids: **(5 L)**

The types of matter, classification of solids, close packing of atoms; Voids in closest packings; Radius ratio rule, Structure of ionic Crystals; Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX_2, spinel structure, perovskite 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,Chemical vapour Transport, Choosing a method for solids.

Books:

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

Section II : Analytical techniques for solids (30 lectures)

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 sin2□□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 :

1. Thermal Analysis-Wendland
2. Instrumental Methods of Analysis-G-Chatwal and S. Anand (Himalaya Publication;1988)
3. Catalysis: Principles & Applications-B.Viswanathan,S.Savasankar and A.V.Ramaswamy (Narosa Publication; 2004). (For XRD part)
4. Solid State Chemistry: An Introduction-Lesley Smart and Elaine Moore (2nd Edition, Chapman and Hall, 1996).
5. Crystallography and its applications-L.S.DentGlasser (Van Nostrand, 1977)
6. Handbook of Applied Solid State Spectroscopy-D.R.Vij (Springer Science, 2006).
7. Optical Properties and Spectroscopy of Nanomaterials-Jin Zhong Zhang (World Science Publication, 2004).
8. Solid Chemistry: techniques-A.K.Cheetham and P.Day (Oxford University Press, 1987).
9. Crystal Structure Analysis- M.J.Buerger (John Wiley, 960).
10. Physical Methods for Chemists-R.S.Drago (2^{nd} Edition, Saunders).

Other Books:

1. Element of X-ray Diffraction-B.D.Cullity (1967)
2. The Synthesis and Characterization of Inorganic Compounds-W.L.Jolly (Prentice Hall, 1970).
3. Synthesis and Techniques in Inorganic Chemistry-R.J.Angelias (2nd Edition, Saunders, 1977).
4. Structural Methods in Inorganic Chemistry –E.A.V.Ebsworth,D.W.H.Rankin and S.Cradock (Blackwell Scientific Publication, 1987).

IC 326: Inorganic Reaction Mechanism and Photochemistry (4Credits, 60L)

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: SN1, SN2 SNICB 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 and J. 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:

1. 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).
2. Mechanism of Inorganic Reactions in Solution – An Introduction, D. Benson, McGraw – Hill
   Chapt.15, p.465, (1968).
3. 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).
4. 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 nondonor 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:

1. Inorganic Chemistry, D.F.Shriver, P.W.Atkins and C.H.Langford, Oxford, 2nd. edn. 1994.
2. An Introduction to Inorganic Chemistry by K.F.Purcell and J.C.Kotz, Saunders 1990, Chapter 14.
3. Comprehensive Coordination Chemistry, Vol.1. G Wilkinson (Ed) Wiley, New York, 1967.
4. Inorganic Chemistry by J.E.Huheey, E.A.Keiter and R.L.Keiter 4th edn. Harper Collins, 1993
5. Mechanisms of Inorganic Reactions, by C.F.Basolo and R.G.Pearson, Wiley, New York, 1967.

Practicals:

IC 328: Experiments in Inorganic Chemistry I (4Credits, 9 weeks)

IC 329: Experiments in Inorganic Chemistry II (4Credits, 9 weeks)

SEMESTER- IV

IC 420: Inorganic polymers, clusters and Heterogeneous catalysis: (4Credits, 60L)

Section I : Inorganic Polymers (30 lectures)

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

2. Inorganic polymer characterization: Average molecular masses (Mn, Mw) 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) Chapter 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.

7. 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:

1. Heterogeneous catalysis principles and application, G.C.Bond.
2. Introduction to zeolite science and practice, H. Van Bekkum, E. M. Flanigen, P. A. Jacobs and J. C. Jansen (Elseviver Pub. Amsterdam, 2001)
3. Catalysis: Principles and Applications, B.Vishwanathan, S. Sivasankar and A.V.Ramaswamy (Narosa Pub. House, New Delhi, 2004)
4. Advanced material in catalysis, James J. Burton and Robert L. Garten (Academic press, New York, 1977)

IC421: Solid state chemistry of Inorganic Materials (4Credits, 60L)

Section I : (30 lectures)

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, classification of 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 YBa2Cu3O7-□□oxide, Fullerenes, intermetallic superconductors, synthesis of superconductors. Application of superconducting materials.

Section II: (30 lectures)

1. Ceramic Materials
Classification of ceramics, dielectric properties and polarization properties 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. Applications of composite materials.

3. Advanced 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 cementitious 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:

1. Introduction to Solids - L. V. Azaroff (Tata MaGraw Hill)
2. Materials Science and Engineering – V. Raghavan (2nd Edition 1980)
3. Elements of Materials Science and Engineering – Van Vlack (5th Edition, Wiley 1988)
4. Nature and Properties of Engineering Materials – Z. D. Jastrazebski (John Wiley Sons, 1989)
5. Principles of Materials Science and Engineering – William F. Smith (Wiley, 1991)
6. Insight into Speciality Inorganic Chemicals – David Thompson (The Royal Society of Chemistry, 1995 chapter 13 and 14)

OPTIONAL COURSES (any one)

IC 425: Industrial inorganic chemicals and medicine chemistry (4Credits, 60L)

Section I: Inorganic Application in Industry (30 lectures)

1. 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).

2. Industrial gases: **(6L)**

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

3. 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.

4. 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.

5. 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.

6. 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 lectures)

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

□- Particle emitting radionuclides
□- 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.

IC 426: Advanced Techniques in Inorganic chemistry (4Credits, 60L)

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. Mass Spectrometry: (Ref.2: p.465-507) (Ref. 1:p.606-664) **(7L)**
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

4. Surface characterization by spectroscopy and microscopy (Ref.1: p.647-682) **(8L)**
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.

5. Particle size determination (Ref. 1: p. 1038-1051) **(6L)**
Introduction to particle size analysis , Low-angle Laser, light scattering , Dynamic light scattering , Photosedimentation.

6. Environmental sampling and analysis (Ref.3: ch.26,p.712) **(8L)**
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.

7. 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.

8. 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.

9. 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

10. LASER spectroscopy in Inorganic Complexes (Ref.5 Chap.6 p. 308-319 and 332-48) **(5L)**
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. Analytical Chemistry (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 Interscience Publication, 2013)

IC 427 Research Project (4Credits, 9 weeks)

Courses which can be opted by students from outside departments:

Elective courses Semester-III

IC 325: Frontiers in Material Science and Analytical Techniques for Solids (4Credits, 60L)

Section I Frontier's in material science (30 lectures)

1. The Structure of solids: **(5 L)**

The types of matter, classification of solids, close packing of atoms; Voids in closest packings; Radius ratio rule, Structure of ionic Crystals; Ionic Crystals with stoichiometry MX, Ionic Crystals with stoichiometry MX_2, spinel structure, perovskite 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,Chemical vapour Transport, Choosing a method for solids.

Books:

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

Section II : Analytical techniques for solids (30 lectures)

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 sin2□□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 :

11. Thermal Analysis-Wendland
12. Instrumental Methods of Analysis-G-Chatwal and S. Anand (Himalaya Publication;1988)
13. Catalysis: Principles & Applications-B.Viswanathan,S.Savasankar and A.V.Ramaswamy (Narosa Publication; 2004). (For XRD part)
14. Solid State Chemistry: An Introduction-Lesley Smart and Elaine Moore (2nd Edition, Chapman and Hall, 1996).
15. Crystallography and its applications-L.S.DentGlasser (Van Nostrand, 1977)
16. Handbook of Applied Solid State Spectroscopy-D.R.Vij (Springer Science, 2006).
17. Optical Properties and Spectroscopy of Nanomaterials-Jin Zhong Zhang (World Science Publication, 2004).
18. Solid Chemistry: techniques-A.K.Cheetham and P.Day (Oxford University Press, 1987).
19. Crystal Structure Analysis- M.J.Buerger (John Wiley, 960).
20. Physical Methods for Chemists-R.S.Drago (2^{nd} Edition, Saunders).

Other Books:

5. Element of X-ray Diffraction-B.D.Cullity (1967)
6. The Synthesis and Characterization of Inorganic Compounds-W.L.Jolly (Prentice Hall, 1970).
7. Synthesis and Techniques in Inorganic Chemistry-R.J.Angelias (2nd Edition, Saunders, 1977).
8. Structural Methods in Inorganic Chemistry –E.A.V.Ebsworth,D.W.H.Rankin and S.Cradock (Blackwell Scientific Publication, 1987).

Semester-IV

IC 425: Industrial inorganic chemicals and medicine chemistry (4Credits, 60L)

Section I: Inorganic Application in Industry (30 lectures)

1. 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).

2. Industrial gases: **(6L)**

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

3. 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.

4. 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.

5. 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.

6. 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
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6. New Trends in Green Chemistry (2nd Edition)-V.K.Ahluwalia and M.Kidwai (Anamaya Publishers, 2007)

Section II: Inorganic Application in Medicine (30 lectures)

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
□- Particle emitting radionuclides
□- 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.

IC 426: Advanced Techniques in Inorganic chemistry (4Credits, 60L)

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. Mass Spectrometry: (Ref.2: p.465-507) (Ref. 1:p.606-664) **(7L)**
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

4. Surface characterization by spectroscopy and microscopy (Ref.1: p.647-682) **(8L)**
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.

5. Particle size determination (Ref. 1: p. 1038-1051) **(6L)**
Introduction to particle size analysis , Low-angle Laser, light scattering , Dynamic light scattering , Photosedimentation.

6. Environmental sampling and analysis (Ref.3: ch.26,p.712) **(8L)**
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.

7. 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.

8. 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.

9. 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

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

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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. Analytical Chemistry (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 Interscience Publication, 2013)