

M Sc Semester III Inorganic Chemistry

CHE2301IC

Bonding and Electronic Spectroscopy [3 credits]

Unit I: *Energy states of transition metal ions and electrostatic perturbation: [1 credits]*

Unit II: *Covalent bonding in metal complexes and their electronic spectra:[2 credits]*

Unit I: *Energy states of transition metal ions and electrostatic perturbation: [15hr]*

Effect of symmetry of ligand field on splitting of d orbitals, octahedral perturbation and calculation of d orbital energies, significance of Dq , factors affecting crystal field splitting, spectrochemical series, splitting of d orbitals in T_d and square planar fields. Jahn-Teller Theorem, static and dynamic Jahn-Teller distortion and distortion in excited states. Limitations of crystal field theory, Nephelauxetic effect, other evidences of metal and ligand orbital overlap, ACFT and LFT.

Unit II: *Covalent bonding in metal complexes and their electronic spectra: [30hr]*

Symmetry aspects of valence bond theory as applied to metal complexes, Molecular orbital theory, composition of ligand group orbitals, and π molecular orbitals, charge transfer spectra.

Selection rules for d-d transitions. Effect of weak fields on RS terms in Octahedral and tetrahedral complexes, Orgel diagrams, Strong field cases and correlation diagram. Tanabe-Sugano diagrams. Spectra of distorted octahedral and square planar complexes. Calculation of transition energy.

Spectral properties of Lanthanide and actinide complexes, f-f transitions, f-d transitions and their sensitivity to ligand environment.

Optical activity of metal complexes and complexes with chiral ligands. Circular dichroism and optical rotatory dispersion spectra of the metal complexes.

Reference Books:

1. Inorganic Chemistry, K.F.Purcell and J.C. Kotz, W.B. Saunders, Philadelphia, (1997)
2. Inorganic Chemistry : Structure and reactivity , James E. Huheey. Harper and Row Publishers, New York, (1983 & 2000)
3. Coordination Chemistry , A.E. Martell Vol. I, Van Nostrand-Reinhold, (1971)
4. Spectroscopy in Inorganic Chemistry : Vol I and II, J.R. Ferraro and C.N.R Rao. Academic Press, London , (1970 & 1971)
5. Inorganic Electronic spectroscopy , A.B. P.Lever, Elsevier, London, (1984)
6. Transition metal Chemistry , R.L. Carlin Vol. 1 to 5, Academic Press, London, (1966)
7. Absorption spectra and chemical bonding in complexes , C.K. Jorgenson Pergamon, Elmsford, New York
8. Inorganic Chemistry , D.F. Shriver, P.W. Atkins and C.H. Langford. Oxford Univ. press, 2nd Edn. (1994), New York.
9. Comprehensive coord. chem.I, G.Wilkinson(Ed.), Vol.1, Elsevier, (1987)
10. Comprehensive coord. chem. II, C.J.McCleverty,(Ed.) Vol. 1-10, Elsevier, (2003)
11. Progress in Inorganic Chemistry , F.A. Cotton & S.J. Lippard (Eds.) Vol. 1 - 37. Academic Press. (1959 & 1966)
12. Coordination Chemistry , D. Banerjee, Tata McGraw Hills, (1993)
13. Theoretical Inorganic chemistry , Day and Selbin, East West Press, (1985)

14. Advanced Inorganic Chemistry , F.A. Cotton and G. Wilkinson (First, Second, Third and Fifth Edition). Interscience. (1988)
15. Chemical applications of group theory, F. A. Cotton, (3rd edition), Wiley. (1990)

M Sc Semester III Inorganic Chemistry

CHE2302IC Inorganic Reactions [3 credits]

Unit I: *Substitution reactions and reactions of coordinated ligands: [1 Credit]*

Unit II: *Mechanisms of redox processes & reactions of coordinated ligands: [1 Credit]*

Unit III: *Inorganic Photochemistry-1: [1 Credit]*

Unit I: Substitution reactions and reactions of coordinated ligands:

Metal and ligand substitution reactions: Metal substitution. Substitution in octahedral complexes, A, D and I mechanisms and associated energetics. Aquation and base hydrolysis, stereochemical changes, isomerisation and racemisation. Fuoss- Eigen equation and factors determining A or D mechanisms, lability and inertness of complexes. Substitution in square planar complexes, "Trans effect" and its theories, "cis-effect". Designing synthetic routes to cis-platin and other complexes of Pt group elements.

Unit II: Mechanisms of redox processes & reactions of coordinated ligands:

Mechanism of Atom transfer processes, halogen, oxo- and hydride transfer reactions. Electron transfer reactions, classification.

Outer-sphere electron transfer mechanisms, chemical activation, Marcus theory, cross-reactions and thermodynamics.

Inner-sphere electron transfer mechanisms, kinetics, effect of the nature of metal and ligands, bridging group effects.

Reactions involving N_2 , H_2O_2 and molecular oxygen.

Reactions of coordinated Ligands: Acid dissociation, hydrolysis of amino acid esters, peptides, proteins and nucleotides, aldol condensation, substitution, amine exchange, trans amination, thermodynamic and kinetic template effects, metal assisted macrocyclization.

Metal-ligand redox reactions.

Unit III: Inorganic Photochemistry-1:

Excited states of metal complexes: intraligand, ligand field, charge transfer and delocalized states.

Charge transfer excited states and redox processes, communication between excited states, radical-pair models.

Ligand field chemistry of excited states: rules for photosubstitution, photoaquation and ligand exchange reactions, photoisomerization, photoracemization and photoanation. Doublet hypothesis, role of quartet excited states, photosubstitution mechanism. Photochromism.

Metal complex sensitizers, photochemical properties of $[Ru(bipy)_3]^{2+}$ and its excited states, oxidative quenching by methyl viologen, chemically modified viologens and non-viologens, reductive quenching, water photolysis using metal complex sensitizers.

Application of redox processes of electrochemically excited states for catalytic purposes, water photolysis, nitrogen and CO_2 reduction, photocatalysts for solar energy conversion.

Reference Books :

1. Inorganic Chemistry, K.F.Purcell and J.C.Kotz,WBSaunders, Philadelphia, (1997)
2. Inorganic reaction mechanism , Basolo and R.G. Pearson.
John Wiley, New Delhi .(1974)
3. Inorganic Chemistry : Structure and reactivity , James E. Huheey.
Harper and Row Publishers, New York, 4th Ed., (1993)
4. Transition metal Chemistry , R.L. Carlin Vol. 1 to 5, Academic Press, London.
5. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and C.H. Langford,
Oxford Univ. press. (1990)
6. Comprehensive coordination chemistry, G. Wilkinson (Ed.) Vol. 1,Elsevier, (1987)
7. Progress in Inorganic Chemistry, F.A. Cotton & S.J. Lippard (Eds.) Vol.1 - 47. Academic Press.
8. Coordination Chemistry, D. Banerjee, Tata McGraw Hill, (1993).
9. Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson (second, third, fifth and sixth Editions), (1966), (1992), (1999) (2003)
10. Mechanisms of Reactions at transition metal sites, R.A. Henderson
Oxford Sci. Publication, (1995)
11. Concepts of Inorganic Photochemistry, A.W.Adamson and P.D. Fleischauer,
Wiley Interscience, (1975)
12. Fundamentals of Photochemistry, K.K. Rohatagi-Mukherjee. Wiley-Eastern, (1986)
13. Introduction to Modern Inorganic Chemistry, W.E. Porterfield, Addison-Wesley, (1984)
14. The Chemistry of excitation at interfaces, J.K. Thomas, ACS, (1984)
15. Principles and applications of organotransition metal chemistry, J.P. Collman, L. S. Hegedes, J. R. Norton and R. G. frike.
16. Fluorescence quenching theory and applications. Maurice R. Eftink.
17. Spectroscopic Analysis of Drugs- Nucleic Interactions. Geoffrey Dougherty and William J.Pigra.
18. Principles of fluorescence spectroscopy. Lakowicz.

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M Sc Semester III Inorganic Chemistry

CHE2303IC Bioinorganic Chemistry-1 [3 credits]

Unit I : Metal ions in Biology, Essentiality and Toxicity: [1 Credit]

Unit II : Storage and Transport of Metal ions, Interaction with Nucleic acid: [1 Credit]

Unit III : Photosynthesis and Mo enzymes[1 Credit]

Unit I : Metal ions in Biology, Essentiality and Toxicity

Elementary cell biology, Occurrence of inorganic elements in biological systems, Bulk and trace metal ions, Beneficial and toxic effects of metal ions, Emergence of Bioinorganic Chemistry.

Coordination sites in biologically important ligands, ternary complexes as models for active sites in metallo-proteins.

Role of alkali metal ions in the biological systems, Ionophores and passive transport, Sodium pump and active transport.

Structural role of calcium, intra and extra cellular calcium binding proteins. Transport of calcium across Sarcoplasmic Reticulum.

Unit II : Storage and Transport of Metal ions, Oxygen and electron transport:

Transport of dioxygen: Oxygen transport by heme proteins, hemoglobin and myoglobin. Nonheme oxygen carriers, hemerythrin, hemocyanin and hemovanidin. Model synthetic complexes of iron and copper as oxygen carriers.

Iron transport by Transferrin and Siderophores, Ferritin in iron storage, Ceruloplasmin.

Glucose metabolism and storage, Bioenergetics and ATP cycle

Unit III: Photosynthesis and Mo enzymes:

Photosystem I and II, light and dark reactions, structure of Mn₄ cluster and mechanism of water splitting. Model system for water splitting and CO₂ reduction. Photochemistry of Ru(bipy)₃³⁺ and metal porphyrins.

Nitrogenases - Biological nitrogen fixation, structure and activity of Fe-Mo nitrogenase, other nitrogenases, model systems

Biological role and mechanistic aspects of xanthine oxidase and sulfite oxidase.

Reference Books:

1. Inorganic Chemistry of Biological Processes , M.N. Hughes, (1975) John Wiley, London
2. Bio-inorganic Chemistry An introduction, E. Ochi Thomas, Soringfield, Allyn and Bacon, Inc. -(1977.)
3. Inorganic Biochemistry, G.L. Eichhorn Vol. I & II,(1973) Elsevier, London
4. Bio-inorganic Chemistry, R.W. Hay – R.W. Hay, Ellis Horwood Ltd Publ. Chichester 1984
5. Inorganic Chemistry, J.E.Huheey, 4th Edition,(1993) Addison–Wesley, Singapore
6. Metal ions in Biological Systems Ed by H. Sigel Vol I to XIX, Marcel Dekker, Basel
7. Principles of Bio Inorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.(1994)
8. Facets of coordination chemistry Ed by B.V. Agarwala & K.N. Munshi, World Scientific, Singapore, NJ, London.
9. Bioinorganic Chemistry , Bertini, Gray, Lippard, & Valentine

Viva books pvt ltd (1998)

10. BioInorganic Chemistry an introduction by J.A. Cowan, Wiley-VCH.

11. Advanced Inorganic Chemistry , F.A. Cotton and G. Wilkinson (fifth Edition).(1999)

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M Sc Semester III Inorganic Chemistry

Practical Courses

CHE2304IC (4 credits)

1. Analysis of complex materials (ores, alloys and composites). (5)
 2. Preparation and characterization of binuclear and mononuclear complexes. (5)
 3. Preparation of fine chemicals and pigments. (4)
 4. Solvent extraction: separation of binary mixtures. (3)
 5. Ion exchange: separation of binary mixtures. (3)
 6. Fertiliser analysis: (N, P, K).
 7. Water analysis (hardness, dissolved solid, COD,BOD, analysis of anions, metal ions).
 8. Gas chromatographic separations.
 9. Separation and identification of aminoacids or metal ions by TLC and PC.
 10. Use of computers in
 - (a) exploring the functions, plots, curve/ line fitting,
 - (b) Determination of stability constants of complexes
 - (c) Determining rates of reactions
 - (d) Application of structure drawing softwares.
 - (e) Calculation of wave function and propbabilities
 - (e) Analysing the data of magnetic measurements
 - (f) Use of Semi-empirical and quantum mechanical calculations (Introductory level)
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M Sc Semester III Inorganic Chemistry

Practical Courses

CHE2305IC(4 credits)

1. Analysis of complex materials (ores, alloys and composites). (5)
 2. Preparation and characterization of binuclear and mononuclear complexes. (5)
 3. Preparation of fine chemicals and pigments. (4)
 4. Solvent extraction: separation of binary mixtures. (3)
 5. Ion exchange: separation of binary mixtures. (3)
 6. Fertiliser analysis: (N, P, K).
 7. Water analysis (hardness, dissolved solid, COD,BOD, analysis of anions, metal ions).
 8. Gas chromatographic separations.
 9. Separation and identification of aminoacids or metal ions by TLC and PC.
 10. Use of computers in
 - (a) exploring the functions, plots, curve/ line fitting,
 - (b) Determination of stability constants of complexes
 - (c) Determining rates of reactions
 - (d) Application of structure drawing softwares.
 - (e) Calculation of wave function and propbabilities
 - (e) Analysing the data of magnetic measurements
 - (f) Use of Semi-empirical and quantum mechanical calculations (Introductory level)
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M Sc Semester III Inorganic Chemistry

CHE2303IE Ionic Solids [2 Credits]

Unit I: Structures of Ionic solids:[1credit]

Unit II: Defects, Electrical and Magnetic properties of solids:[1 credit]

Unit I: Structures of Ionic solids:

Ionic Solids: Amorphous and crystalline solids, types of water in crystals, Lattice energy, Madelung constant, Kapustinskii equation, Born-Haber cycle.

Close packing, radius ratio rules, calculation of hole size in trigonal planar, tetrahedral, octahedral and cubic sites, Structures of binary, bi-, tri-, terta- and pentaatomic molecules, Adamantine and layer lattice structures.

Ternary and mixed oxides: Structures and comparison of corundum, Ilmenite, Perovskite, Olivine, spinels, inverse spinels, valency disordered spinels, structural relationship between iron oxides. Ferrites- Cubic ferrites of the spinel and garnet type, hexagonal ferrites.

Unit II: Defects, Electrical and Magnetic properties of solids:

Defects in stoichiometric and nonstoichiometric compounds, experimental methods for detection of defects, consequences of defects – colours in ionic solids, ionic conductivity, solid electrolytes. Magnetic and electrical properties of solids, Hall effect, Seebeck and Peltier effects, effect of stress and strain on electrical properties.

Ferroelectric, pyroelectric and piezoelectric materials.

Inorganic chemicals and metals in electronics industry: materials for electronics, elemental and compound semiconductors, processing methods for electronic materials (sputtering, CVD, photolithography, LB films), thick films and packaging materials (rectifiers, transistors, capacitors, MOSFET), chemical sensors, Non linear optical materials.

Reference Books:

1. Structural principles of Inorganic Chemistry, W.E. Addison, Wiley, New York.
2. Semiconductors , N.B. Hanay, Reinhold, New York.(1959)
3. Modern aspects of solid state Chemistry, C.N.R. Rao, Plenum Press, NY (1970)
4. Solid State Chemistry, C.N.R. Rao, Dekker, New York (1974)
5. Phase transitions in solids, C.N.R. Rao and K.J. Rao, McGraw Hill, New Delhi.
6. Ionic Crystals and lattice defects and non-stoichiometry, N.N. Greenwood, Butterworths, U.K.(1970)
7. Structure and bonding in solid state Chemistry, M.F.C.Ladd, Ellis Horwood Ltd., London (1979)
8. Modern Aspects of Inorganic Chemistry , Emeleus and Sharpe. Routledge, England , New Delhi Universal Book (1977)
9. Treatise on Solid state Chemistry Vol. 4 , N.B. Hannay, Plenum Press, (1996)
10. Introduction to super conductivity , C.N. R. Rao, Wiley eastern(1992)
11. Principle the “Solid State” H.V.Veer, John Willey, New Delhi, (1993)
12. Structural Inorganic Chemistry, A.F. Wells., Oxford University Press. (1962) (1990)
13. Solid State Chemistry and its applications, A,R, Welf, John Willy, New York, (1998).

M Sc Semester III Inorganic Chemistry

CHE2304IE

Speciality Inorganic Chemicals [2 Credits]

Unit I: Silicates, Zeolites and Speciality Inorganic chemicals-1: [1 credit]

Unit II: Metal alkoxides, semiconducting oxides and superconductors: [1 credit]

Unit I: Silicates, Zeolites and Speciality Inorganic chemicals-1:

Glassy state and structures of glasses, network formers and network modifiers, Zachariassen rule, modification of properties by variation in composition and structure, Advanced cementitious materials.

bioactive ceramics and bioactive glasses.

Fast ion conductors and their applications- Types of ionic conductors, mechanism of ionic conduction, diffusion superionic conductors, phase transitions and mechanism of conduction in superionic conductors, applications.

Ionic liquids and their applications.

Unit II: Metal alkoxides, semiconducting oxides and superconductors:

Synthesis, stability and reactivity of metal alkoxides. Double alkoxides, mixed alkoxides. Use of alkoxides as reagents in organic synthesis. Alkoxides as precursors to mixed oxides.

Semiconducting oxides and their applications.

Hard and soft magnetic materials, magnetic recording materials and magnetic switching devices.

Introduction to superconductivity, mechanisms of superconduction, types of superconductors, cuprate superconductors, structures of Y-Ba-Cu-O and related systems. Synthesis, Chemical properties and structures of high T_c superconductors, applications.

Reference Books:

1. Structural principles of Inorganic Chemistry, W.E. Addison, Wiley, New York.
2. Semiconductors, N.B. Hanay, Reinhold, New York.(1959)
3. Modern aspects of solid state Chemistry, C.N.R. Rao, Plenum Press, NY (1970)
4. Solid State Chemistry, C.N.R. Rao, Dekker, New York (1974)
5. Phase transitions in solids, C.N.R. Rao and K.J. Rao, McGraw Hill, New Delhi.
6. Ionic Crystals and lattice defects and non-stoichiometry, N.N. Greenwood, Butterworths, U.K.(1970)
7. Structure and bonding in solid state Chemistry, M.F.C. Ladd, Ellis Horwood Ltd., London (1979)
8. Modern Aspects of Inorganic Chemistry, Emeleus and Sharpe. Routledge, England, New Delhi Universal Book (1977)
9. Treatise on Solid state Chemistry Vol. 4, N.B. Hannay, Plenum Press, (1996)
10. Introduction to super conductivity, C.N. R. Rao, Wiley eastern(1992)
11. Principle the "Solid State" H.V. Veer, John Willey, New Delhi, (1993)
12. Insights into speciality inorganic chemicals, Ed. D. Thompson, RSC.(1995)
13. Structural Chemistry of Silicate, Friedric Liebau, Springer, Verlag (1985)
14. The Chemistry of excitation at interfaces, J.K. Thomas, ACS, (1984)

M Sc Semester III Inorganic Chemistry

CHE2301IE Supramolecular Chemistry [2 credits]

Unit I: Supramolecular chemistry and molecular recognition:[1 credit]

Unit II: Supramolecular devices:[1 credit]

Unit I: Supramolecular chemistry and molecular recognition:

Concept of supramolecular chemistry, supramolecular building blocks and spacers, molecular recognition and host-guest interaction, molecular receptors for different types of ions and molecules. Design and synthesis of coreceptor molecules and multiple recognition. Spherical and tetrahedral recognition.

Organometallic and macrocyclic receptors: corands, cryptands, catenands, spherands, calixarenes and cyclodextrins, ferrocene, cobaltocenium, and other metallocene based receptors.

Unit II: Supramolecular devices

Ditopic and polytopic receptors, metal assisted molecular and supramolecular assemblies. Supramolecular magnetic devices, supramolecular ionic and switching devices, Molecular wires.

Supramolecular reactivity and catalysis, models for ATPase and phosphorylation enzymes. Transport processes and carrier design. Supramolecular photochemistry, self organization and molecular assembly in molecular architecture.

Biosensors.

Reference Books:

1. Supramolecular Chemistry, J. -M. Lehn, VCH publ. (1995)
 2. Chemistry of Macrocyclic compounds, L. F. Lindoy, Cambridge Univ. Press,(1990).
 3. Transition metals in supramolecular chemistry, Luigi Fabbrizzi, Antonio Poggi, Kluwer, 1994.
 4. Encyclopedia of Supramolecular Chemistry, 2 Volume Set,edited by Jerry L. Atwood and Jonathan W. Steed
 5. Introduction to supramolecular chemistry By Helena Dodziuk, Kluwer Acad Publ, 2002
 6. <https://people.ifm.liu.se/thoed/TFYA30/Lehn%28Nobel%29.pdf>
 7. http://nobelprize.org/nobel_prizes/chemistry/laureates/1987/lehn-lecture.pdf
 8. Supramolecular Chemistry, J. W. Steed, J. L. Atwood, John Wiley, (2002)
 9. Principles and Methods in Supramolecular Chemistry, H. -J. Schneider, A Yatsimirsky, John Wiley, (2000).
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M Sc Semester III Inorganic Chemistry

CHE2302IE

Spectroscopic and Microscopic methods [2 Credits]

Unit I: Atomic spectroscopies, scattering and diffraction methods:[1 credit]

Unit II : MS,EM and Nuclear spectroscopies:[1 credit]

Unit I: Atomic spectroscopies, scattering and diffraction methods:

Applications of Atomic emission, Atomic absorption and Atomic fluorescence spectrometry, recent advances (e.g. resonant ionization and laser enhanced ionization spectroscopy).

Radiation scattering techniques: Nephelometry, Turbidimetry, Theory, instrumentation and applications of Raman spectrometry with reference to resonant, linear, nonlinear techniques.

X-ray Methods: Theory, instrumentation and applications of XRF, ESCA and Auger.

X-ray Diffraction: Single crystal X-ray diffraction and powder x-ray diffraction methods

Unit II : MS,EM and Nuclear spectroscopies:

Mass Spectrometry: Use of FAB, ESI and MALDI in the molecular and bio-molecular characterization.

Electron microscopy: Use of SEM, TEM and AFM in characterizing soft materials, nano particles and surface analysis.

NQR spectroscopy and its applications.

Mossbauer spectroscopy: isomer shift, isotropic and anisotropic electronic fields, effects of nuclear quadrupole on Mossbauer spectra.

Reference Books :

1. Introduction to instrumental analysis , Robert Braun, McGraw Hill Co. International Ed. (1987)
2. Fundamentals of analytical chemistry , D.A. Skoog, D.M. West & F.J. Holler, Saunders College Pub. 7th Edition.(2001)
3. Principles of Instrumental Analysis , D.A. Skoog, F. J. Holler, & T. A. Neimen Saunders College Pub. 5th Edition. (1998)
4. Investigation of Molecular Structure , B.C. Guilbert, ELBS, 2nd Edition (1975)
5. Thermal Analysis , T. Daniels, Kogan Page (1975.)
6. Differential Thermal Analysis , M.I. Pope & M.D. Judd, Hyden & Son Ltd. (1975).
7. Principles of applications of electrochemistry. Crow. D.R. 3rd Ed. (1998)
8. Electrochemical Methods, A. J. Bard and L.F. Faulkner, Wiley, New York. (2004)
9. Modern Polarographic methods in Analytical Chemistry, A. M. Bond, marcel Dekker, New York. (1980)
10. Principles of electroanalytical Methods, T. Riley and C. Tomlinson (Anal. Chem by open learning), John Wiley and sons.(1987)

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M Sc Semester IV Inorganic Chemistry

CHE2401IC

Magnetism and Spectroscopy [3credits]

Unit I: *Magnetic properties of transition metal ions and lanthanides* : [1 Credit]

Unit II: *ESR spectroscopy*: [1 Credit]

Unit III: *Vibrational spectroscopy*: [1 Credit]

Unit I: Magnetic properties of transition metal ions, complexes and lanthanides:

Introduction to Magnetochemistry: Types of magnetism and temperature dependence of magnetic susceptibility, Curie and Curie-Weiss laws, Measurement of magnetic susceptibility by Gouy method, Faraday method and Evan's NMR method.

Types of magnetism in transition metal complexes, spin orbit coupling, quenching of orbital moment in metal complexes, Temperature independent paramagnetism. Spin paired and spin free equilibria in complexes.

Magnetic properties of polynuclear complexes, M-M direct interaction and super exchange through small bridges, long-range magnetic interactions, factors affecting the spin exchange in multinuclear species, molecular magnetic materials.

Magnetic properties of lanthanides.

Unit II: ESR spectroscopy:

ESR spectra of metal complexes: Zeeman interaction and energy levels, g factor, Ligand field effects, dipolar coupling, Hyperfine coupling and A parameter, super-hyperfine coupling. Orbital moment quenching and g values, Anisotropy in g and A values.

ESR spectra of multielectronic ion complexes. Zero field splitting and Kramer's degeneracy, ESR spectra of d^1 to d^9 metal ions, ESR spectra of binuclear metal complexes. Some examples of biomolecules. Introduction to ENDOR and ESEEM.

Unit III: IR, Raman and NMR spectroscopy:

Infrared and Raman spectral studies of simple inorganic compounds and metal complexes: selection rules. Active and degenerate vibrations, effect of functionalization and symmetry change on IR and Raman spectra. Changes in ligand vibrations on coordination with metal ion. Metal-ligand atom vibrations.

Proton, fluorine and phosphorous NMR of Inorganic compounds, Diamagnetic metal complexes, contact and pseudo-contact shifts in paramagnetic complexes, Lanthanide complexes as shift reagents.

Reference Books :

1. Transition metal Chemistry , R.L. Carlin Vol. 1 to 5, Academic Press, London, (1966)
2. Infrared and Raman Spectra of Inorganic and Coordination compound, K. Nakamoto, John Wiley, 3rd Edn. (1978)
3. Comprehensive coordination chemistry I, G.Wilkinson(Ed.)Vol.1, Elsevier,(1987)
4. Comprehensive coordination chemistry II, C.J. McCleverty,(Ed.) Vol. 1-10, Elsevier, (2003)
5. Progress in Inorganic Chemistry, F.A.Cotton & S.J.Lippard (Eds.), Vol. 1-37, Academic Press, (1959 & 1966)
6. Spectroscopy & structure of metal chelate compound. K. Nakamoto & P.J.M. Arthy, John Wiley (1997)
7. Elements of Magnetochemistry, A. Syamal and R.L.Dutta,
8. Magnetochemistry, Mabbs and Machin,
9. Magnetochemistry, R. L. Karlin, Springer-Verlag. Berlin, (1986)
10. Chemical applications of group theory, F. A. Cotton, (3rd edition), Wiley. (1990)
11. ESR spectroscopy, Goodman and Rayner.
12. Transition ion Electron paramagnetic resonance, J. R. Pilbrow, Oxford Sci. Publ. (1990)
13. Mossbauer effect & its applications , V.G. Bhide, Tata McGraw Hill, (1973)
14. Wilkins, CL, Ed. Mass Spectrometry. In Handbook of Instrumental Techniques for Analytical Chemistry; Settle, FA, Ed.; Prentice Hall: Upper Saddle River, NJ, (1997); Section V.
15. De Laeter, JR, Applications of Inorganic Mass Spectrometry, Wiley-Interscience Series on Mass Spectrometry, Desiderio, DM; Nibbering, NMM, Eds.; Wiley Interscience: New York, (2001)
16. Mass Spectroscopy of Inorganic and Organometallic compounds, W. Henderson & J.S. Mcludoe, Wiley (2005).

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M Sc Semester IV Inorganic Chemistry

CHE2402IC

Molecular catalysis and Metalloenzyme reactions [3credits]

Unit I: *Molecular catalysis*: [1 Credit]

Unit II: *Metalloenzymes in Non-Redox reactions*: [1 Credit]

Unit III: *Oxidoreductase and Oxygenase enzymes*: [1 Credit]

Unit I: **Molecular catalysis-1 :**

Catalysis at metal centers, role of ligands and organic groups in deciding the catalytic activity and specificity of metal complexes and organometallics.

Molecular Activation: activation of hydrogen, oxygen, carbon monoxide, alkenes, alkanes, nitric oxide and nitrogen.

Mechanism of metal catalyzed oxidation, homolytic and heterolytic mechanisms, catalytic oxygen transfer, transition metal catalysts for oxidation.

Catalytic hydrogenation, hydrosilation and isomerisation of alkenes and alkynes, cycloaddition and polymerization, olefin metathesis using Grubbs, Schrock and Chauvin catalysts.

Unit I : **Metalloenzymes in Non-Redox reactions:**

Substrate binding and activation by Non redox mechanisms: carboxypeptidaseA, Alkaline phosphatase, carbonic anhydrase, alcohol dehydrogenase, thermolysin.

Activation of nucleotides by metal ions.

Structure and function of various kinase, ATPase and isomerase enzymes

Structure and function of Vitamin B12 and coenzyme, reactions catalyzed by vitamin B12 dependent enzymes with mechanistic details.

Unit II : **Oxidoreductase and Oxygenase enzymes:**

Iron containing enzymes- catalases, peroxidases, methane monooxygenase, Cytochrome P450,

Copper containing enzymes – Types of active copper sites in proteins and their spectral characteristics, Structure and function of Galactose and amine oxidases, superoxide dismutase, tyrosinase, dopamine- β -hydroxylase enzymes. Multicopper oxidases.

Nickel containing hydrogenase enzymes

Electron carriers: Structure and function of blue copper proteins, cytochromes and iron sulphur proteins. Synthetic models.

Reference Books :

1. Progress in Inorganic Chemistry, F.A. Cotton & S.J. Lippard (Eds.) Vol.1 - 47. Academic Press.
2. Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson (second, third, fifth and sixth Editions), (1966), (1992), (1999) (2003).
3. Principles and applications of organotransition metal chemistry, J.P. Collman, L. S. Hegedes, J. R. Norton and R. G. frike,
4. Lanthanides: Chemistry and Use in organic synthesis, Ed. S. Kobayashi, Springer,
5. Experimental methods in Catalytic research, R.S. Anderson, Academic Press, London, (1968)
6. Advanced Materials in Catalysis-Material Science Series, J.J. Burton and R.L. Garten. Academic Press, (1977)
7. Fundamentals of Molecular catalysis, ed. H. Kurosawa and A. Yamamoto, Elsevier(2003).
8. Homogeneous catalysis- understanding the art, Piet W. N. M. van Lecuwan, Kluwer Acad. Publ.
9. Advanced Materials in Catalysis-Material Science Series, J.J. Burton and R.L. Garten. Academic Press.(1977)
10. Spectroscopy in Heterogeneous catalysis , W.N. Delgass, G.L. Haller, R. Kellerman and J.H. Lunsford Academic Press, London. Wiley (1982)
11. BioInorganic Chemistry an introduction by J.A. Cowan, Wiley-VCH.
12. Inorganic Chemistry of Biological Processes, M.N. Hughes, (1975), John Wiley, London
13. Bio-inorganic Chemistry An introduction, E. Ochii, Thomas, Soringfield, Allyn and Bacon, Inc. – (1977.)
14. Inorganic Biochemistry, G.L. Eichhorn Vol. I & II, (1973, Elsevier, London
15. Bio-inorganic Chemistry, R.W. Hay – R.W. Hay, Ellis Horwood Limited Publishers chichester 1984
16. Inorganic Chemistry , J.E. Huheey, 4th Edition, (1993), Addison – Wesley, Singapore
17. Metal ions in Biological Systems Ed by H. Sigel Vol I to XIX, Marcel Dekker, Basel
18. Copper proteins, T. G. Spiro, John Willey, (1981)
19. Principles of Bio Inorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books, 1994)
20. Facets of coordination chemistry Ed by B.V. Agarwala & K.N. Munshi, World Scientific, Singapore, NJ, London.
21. Bioinorganic Chemistry , Bertini, Gray, Lippard, & Valentine, Viva books pvt ltd (1998)

M Sc Semester IV Inorganic Chemistry

CHE2403IC

Organometallic Chemistry and Catalysis [3credits]

Unit I: *Organometallic chemistry*: [1 Credit]

Unit II: *Bonding in Organometallic compounds*: [1 Credit]

Unit III: *Molecular Catalysis-II*: [1 Credit]

Unit I: Organometallic chemistry :

Interaction of organic molecules/ions with transition and non-transition metal ions, classification of organic σ - and π -donors.

Synthesis of organometallic compounds of transition and non-transition elements with σ -donors, chemical vapour deposition, reaction with alkyl halides, metallation, insertion, deinsertion, oxidative addition, reductive elimination and carbonylation reactions.

Organometallic compounds with organic π -donors, synthesis of compounds with acyclic ², ³ and ⁴ and cyclic ⁵ and ⁶ ligands, sandwich compounds, bent metallocenes and compounds with mixed (cyclic and acyclic) donors.

Unit II: Bonding in Organometallic compounds :

Bonding in ¹- complexes, thermodynamic and kinetic stability of M-C σ -bond, “ortho effect”.

Nature of M-C bond in metal-olefin and acetylene complexes, DCD model. Metal carbenes. Structure and bonding in the complexes of 3, 4, 5, and 6 electron donors. Reactivity, magnetism and redox properties.

Fluxional behaviour and dynamic equilibrium, spectral evidence, mechanisms, σ - π rearrangements.

Application of organometallic compounds in organic synthesis: alkylating and arylating agents, Organolithium, organopalladium, organoruthenium compounds, derivatives of zirconocene and other metallocenes in organic synthesis.

Unit III: Molecular catalysis-2 :

Metal complexes in enantioselective synthesis: asymmetric hydrogenation and oxidation of alkenes, catalyst characterization, kinetics and application of these reactions.

Catalyst development and mechanistic aspects of Zeigler – Natta catalysis, Fischer – Tropsch synthesis, water – gas shift reaction, Wacker process, Monsanto process.

Phase transfer and micellar catalysis

Principles of Green Chemistry and Role of catalysis – concept of atom economy, E factors and atom efficiency, typical examples of atom economic reactions and atom un-economic reactions, some specific examples of chemical routes developed using catalysts.

Reference Books :

1. Transition metal organometallic Chemistry, R.B. King, Academic Press, (1995)
2. Organo-metallic compounds, M.L.H. Green, Chapman & Hall, London
3. Organo-metallic Chemistry, A Unified Approach, R.C. Mehrotra and A. Singh, New Age Publisher, (2000)
4. Metallo-organic Chemistry, A.J. Pearson, John Wiley.
5. Organometallics vol. 1 & 2, M. Bochmann, Oxford Univ. press, (1996),
6. Inorganic Chemistry, K.F. Purcell and J.C. Kotz, WB Saunders, Philadelphia, (1997)
7. Inorganic Chemistry : Structure and reactivity, James E. Huheey. Harper and Row Publishers, New York, 4th Ed., (1993)
8. Transition metal Chemistry, R.L. Carlin Vol. 1 to 5, Academic Press, London.
9. Inorganic Chemistry, D.F. Shriver, P.W. Atkins and C.H. Langford, Oxford Univ. press. (1990)
1. Basic Organometallic Chemistry: Concepts, Synthesis and Applications By B D Gupta and A J Elias University Press (India) Pvt. Ltd. (2010)
11. Comprehensive coordination chemistry, G. Wilkinson (Ed.) Vol. 1, Elsevier, (1987)
12. Progress in Inorganic Chemistry, F.A. Cotton & S.J. Lippard (Eds.) Vol.1 - 47. Academic Press.
13. Advanced Inorganic Chemistry, F.A. Cotton and G. Wilkinson (second, third, fifth and sixth Editions), (1966), (1992), (1999) (2003)
14. Principles and applications of organotransition metal chemistry, J.P. Collman, L. S. Hegedes, J. R. Norton and R. G. frike,
15. Lanthanides: Chemistry and Use in organic synthesis, Ed. S. Kobayashi, Springer,
16. Experimental methods in Catalytic research, R.S. Anderson, Academic Press, London, (1968)
17. Advanced Materials in Catalysis-Material Science Series, J.J. Burton and R.L. Garten. Academic Press, (1977)
18. Fundamentals of Molecular catalysis, ed. H. Kurosawa and A. Yamamoto, Elsevier(2003).
19. Homogeneous catalysis- understanding the art, Piet W. N. M. van Lecuwan, Kluwer Acad. Publ.
20. Advanced Materials in Catalysis-Material Science Series, J.J. Burton and R.L. Garten. Academic Press.(1977)
21. Spectroscopy in Heterogeneous catalysis, W.N. Delgass, G.L. Haller, R. Kellerman and J.H. Lunsford Academic Press, London. Wiley (1982)
22. Organometallics- A Concise Introduction, Ch. Eischeinbroich and Salzer-VCH.

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M Sc Semester IV Inorganic Chemistry

Practical Courses

CHE2404IC (3 credits)

CHE2405IC (2 credits)

1. Analysis of Ores and Alloys:
Ores- Pyrolusite, Dolomite, limestone etc
Alloys: Brass, Bronze, Stainless steel etc
 2. Nephelometric determinations (Sulphate/ phosphate).
 3. Use of conductometric titrations for determination of heavy metal ions (Th/Ce/Zr/Cd)
 4. Use of potentiometric / amperometric titrations for determination of metal ions like C and Hg
 5. Study of complex equilibria:
 - a.Determination of Stoichiometry of complex by spectrophotometry/ conductivity method.
 - b.Determination of the protonation constants of ligands and Stability constants of complexes by pH metry.
 6. Catalysis by metal complexes and supported metal complexes.
 7. DNA binding studies (Fluorimetric / spectrophotometric)
 9. Polarographic determinations of metal ions and study of the effect of complexing agents on redox potentials.
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**M Sc Semester IV
Inorganic Chemistry**

CHE2406IC (2 credits)

Comprehensive Viva Voce and Examination

Comprehensive Viva voce Examination by Internal and External Examiners at the end of the IV semester

M Sc Semester IV
Inorganic Chemistry

CHE2407IC (3 credits)

Dissertation

Dissertation work. To be evaluated by a panel of internal examiners at the end of the IV semester.

M Sc Semester IV
Inorganic Chemistry
CHE2408IC (3 credits)

Special Practical and
Assignment

Special practical's:

The concepts studied in the theory will be verified or tested through new skill-enhancing experiments or practicals.

These practical's also include assignments to further improve learning outcomes.

Students undertaking special practical's will be evaluated by a panel of examiners.

M Sc Semester IV Inorganic Chemistry

CHE2401IE

Catalytic materials and Industrial catalysis [2 credits]

Unit I: Catalytic materials and industrial catalysis:- [1 credit]

Unit II: Catalytic materials and industrial catalysis-2: [1 credit]

Unit I: Catalytic materials and industrial catalysis-1

Structural aspects of 1, 2, 3 dimensional and cyclic silicates, aluminosilicates – feldspars, ultramarines and natural zeolites, clay minerals.

Synthesis, structure and characterization of microporous materials- selective Zeolites such as γ -Zeolites, ZSM-5, ZSM-11

Zeolites catalyzed reactions – Electrophilic aromatic substitution, Addition and Elimination, Rearrangement and Isomerization, Cyclization

Zeolites in petrochemical processes- Fluid Catalytic Cracking (FCC), Hydrocracking, Isomerization of n-paraffins, Methanol to Gasoline, Methanol to Olefins

Synthesis, structure and characterization of mesoporous materials- MCM-41, MCM-48, SBA-15, functionalized MCM-41 Reaction catalyzed by functionalized MCM-41 – Michel addition, Aldol reactions

Unit II: Catalytic materials and industrial catalysis-2

Synthesis, structure and characterization of Polyoxometalates (isopolyacids and heteropolyacids) especially molybdates and 12-tungstophosphoric acid, Transition metal substituted Polyoxometalates especially 12-tungstophosphoric acid.

Homogeneous as well as Heterogeneous catalysis with polyoxometalate based compounds- Esterification, etherification, Friedel-Crafts alkylation, Friedel-Crafts alkylation, Oxidation of olefins

Use of oxides, organic polymers, inorganic ion exchangers and mesoporous materials as supports for homogeneous catalysts, Methods for synthesis of supported catalysts, Catalysis by supported Polyoxometalates- Esterifications, Friedel –Crafts alkylation, Oxidation of olefins

Materials for automobile catalysts (synthesis, characterization and mechanism)

Reference Books:

1. Experimental methods in Catalytic research, R.S. Anderson, Academic Press, London, (1968)
2. Advanced Materials in Catalysis-Material Science Series, J.J. Burton and R.L. Garten. Academic Press, (1977)
3. Fundamentals of Molecular catalysis, ed. H. Kurosawa and A. Yamamoto, Elsevier(2003).
4. Homogeneous catalysis- understanding the art, Piet W. N. M. van Lecombe, Kluwer Acad. Publ.
5. Advanced Materials in Catalysis-Material Science Series, J.J. Burton and R.L. Garten. Academic Press.(1977)
6. Spectroscopy in Heterogeneous catalysis , W.N. Delgass, G.L. Haller, R. Kellerman and J.H. Lunsford Academic Press, London. Wiley (1982)
7. Insights into speciality inorganic chemicals, Ed. D. Thompson, RSC.(1995)
8. Structural Chemistry of Silicates, Friedric Liebau, Springer, Verlag (1985)
9. Heteropoly & Isopoly Oxometalates , Michael Thar Pope, Springer Verlag, (1983)

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M Sc Semester IV Inorganic Chemistry

CHE2402IE Medicinal Inorganic Chemistry [2 Credits]

Unit I : Metal ions and complexes in Medicine – I:[1 Credit]

Unit II : Metal ions and complexes in Medicine – II:[1 Credit]

Unit I : Metal ions and complexes in Medicine – I

Metal deficiency and diseases, chelation therapy for metal ion detoxification, Lithium drugs in neurological disorders, gold antiarthritis drugs, pharmacology of auranofin.

Role of metal ions in the action of antibiotics.

Metal ions in clinical diagnosis: MRI agents

Radiopharmaceuticals: Use of Tc, Re, Sm, Sr, Ga, Co, and I isotopes

Unit II : Metal ions and complexes in Medicine – II

Metal- nucleic acid interactions: Coordination, Non-covalent interactions - intercalation and hydrogen bonding, hydrophobic interactions, DNA strand cleavage.

Biological fluorophores. Application of fluorescence quenching in drug-DNA binding studies. DNA binding and mechanistic possibility.

Platinum anticancer drugs, structure activity relationship, mechanism of action, aspects of Pt binding to DNA – kinetics, crosslinking, physical effects and biological consequences,

Nonplatinum antitumor metal complexes: Ru(III) ammine complexes, Antitumor activity, structure activity relationship, DNA binding and cleavage

Anticancer activity of metallocenes,

Structure and chemical properties of streptonigrin and its metal complexes, evidence for formation of ternary complexes involving DNA, antitumor activity and mechanism.

Reference Books:

1. Bio-inorganic Chemistry, R.W. Hay – R.W. Hay, Ellis Horwood Limited Publishers chichester 1984
 2. Metal ions in Biological Systems Ed by H. Sigel Vol I to XIX, Marcel Dekker, Basel
 3. Principles of Bio Inorganic Chemistry, S. J. Lippard and J. M. Berg, University Science Books.(1994)
 4. Facets of coordination chemistry Ed by B.V. Agarwala & K.N. Munshi, World Scientific, Singapore, NJ, London.
 5. Bioinorganic Chemistry , Bertini, Gray, Lippard, & Valentine Viva books pvt ltd (1998)
 6. BioInorganic Chemistry an introduction by J.A. Cowan, Wiley-VCH.
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M Sc Semester IV Inorganic Chemistry

CHE2403IE Industrial Inorganic Chemistry [2 credits]

Unit I: Industrial Metals and Metallurgy: [1 Credit]

Unit II: Heavy and Fine Chemical Industry: [1 Credit]

Unit I: Industrial Metals and Metallurgy: [1 Credit]

Metallurgy of Chromium, Vanadium, Titanium, Molybdenum, Tungsten, Rhodium, Ruthenium, Palladium, Platinum, Silicon, Tin and Lead.

Preparation and Use of Raney Nickel, Monel and Devarda's alloy

Unit II: Heavy and Fine Chemical Industry: [1 Credit]

Industrial acids:

Hydrochloric acid, hydrofluoric acid and perchloric acid.

Industrial bases:

Chloralkali process, manufacture of chlorine, caustic alkalies and soda ash. Corrosion in chloralkali industry and protection.

Industrial oxidizing and reducing agents:

KMnO₄, K₂Cr₂O₇, H₂O₂, Na₂SO₃, Na₂S₂O₃

Industrial Boron, Carbon and Silicon Compounds:

Borax, Boric acid, boron nitride

Carbon black, graphite, calcium carbide, silicon carbide and silicones

Reference Books:

1. Chemical process industries by N.D. Shreeve.
2. applied chemistry for Engineer by Diamont.
3. Industrial poisons and solvents by Jacobs.
4. chemistry of Engineering materials by Jain & Jain.
5. Engineering chemistry by B.K.Sharma.
6. Environmental chemistry by B.K.Sharma.
7. Corrosion, Volume-I, Metal Environment Reactions by L.L.shreir, Newnes Butterworths, London.
8. Corrosion Engineering by Fontana and Greene, McGraw Hill Publication.