

- (vii) Study the phase diagram of a binary system (phenol-water) and the effect of impurities (e.g., NaCl)

Reference Books/ Journals

Mendham, R.C., Denney, J.D., Baines, M. Thomas and Siva Sankar, B. Vogel's Text Book on Quantitative Chemical Analysis, 6/e, Pearson.

Nad, A. K., Mahapatra, B. & Ghosal, A. An Advanced Course in Practical Chemistry, New Central Book Agency, 2007.

Das, S.C. Advanced Practical Chemistry, The World Press Pvt. Ltd., 4th Ed. 2010

Mukhopadhyay, R. & Chatterjee, P. Advanced Practical Chemistry, Books & Allied (P) Ltd., 3rd Ed., 2007.

Maity, S. K. & Ghosh, N. K. Physical Chemistry Practical, New Central Book Agency (P) Ltd. 2012

SEMESTER VII

Chemistry Major/Core Course

Paper Code: CHEM7011

Paper Title: Inorganic General

Credit: 6

Course Objective:

- The objective is to impart into the students (i) theoretical the idea and understanding of chemical bonding and properties through a quantum chemical approach, chemical structures, bonding, stereochemistry and properties of elements and coordination complexes and organometallics, structures and properties of

crystalline and amorphous solids, and (ii) practical knowledge and skills for quantitative estimation and analysis of pyrolusite, dolomite and brass.

Course outcome:

On completion of the course the students will be able to:

- Learn and apply quantum mechanics in understanding chemical bonding with molecular orbital (MO) theory formalism and thereby predict the structures and properties of several homo- and heteronuclear molecules
- Learn and understand the chemistry of elements (nontransition, transition, lanthanides, and actinides) and their compounds of different sizes in varying ligands sites
- Understand and predict the chemical bonding and structures of coordination complexes, and their stereo-chemical, magnetic and spectral properties.
- Analyze and characterize several organometallic compounds in varying ligand systems as well as the interactions therein.
- Ions and their compounds as well as to apprehend their applicability in biological and material sciences
- Understand the fundamentals of ionic, covalent, hydrogen bonded and molecular solids and thereby to explain structural, magnetic and conducting behaviors of different kinds of solids

Theory

Credit: 4

Bonding and properties in chemical system – a quantum chemical approach

15 Hours

The Born-Oppenheimer approximation, the hydrogen molecular ion (H_2^+), Molecular Orbital (MO) theory, Linear Combination of Atomic Orbitals (LCAO), LCAO-MO method, MO of homo- and heteronuclear diatomic molecules, MO of polynuclear AB_n type molecules, Molecular electronic terms, the hydrogen molecule (H_2), electron probability density, dipole moment, Semiempirical treatment of polyatomic molecules: Hückel method of π -MO calculation, Frost diagram of carbocyclic π -systems

Chemistry of elements and Coordination chemistry – structure, bonding, stereochemistry and properties

15 Hours

Chemistry of elements

Elements – structural versatility and related properties; compounds – design and syntheses, isolation, characterization, solution structure, molecular aggregate, crystalline architecture,

spectral, magnetic and catalytic properties and application in chemistry, biology and materials science

Non-transition and transition metal ion homoleptic/heteroleptic and homonuclear/ heteronuclear complexes of different dimensions with varied mono- and polydentate blockers containing carbon, nitrogen, phosphorus, chalcogen, halogen donors with/without mono-/polydentate bridges and counter ions

Inner-transition metals: Ionization energy, electrode potential, metallic and ionic radii, peculiarities in electronic and magnetic properties, coordination chemistry, formation constant, actinyl ion

Coordination chemistry – structure, bonding, stereochemistry and properties

Fundamentals, Orgel diagram, Tanabe-Sugano diagram, ligand symmetry orbital, molecular orbital, spectral properties, Nephelauxetic effect, Racah parameter, vibronic coupling, band broadening, spin-orbit coupling, spin-forbidden transition, intensity stealing, magnetic properties, anomalous and subnormal magnetic moments, lowering of symmetry, electronic, steric, Jahn-Teller and Renner-Teller effects on energy levels, conformation of chelator/congregator, structural equilibrium and implication, Correlation of CFSE with spectroscopy

Organometallic chemistry-I

15 Hours

Overview and striking difference, valence electron count, oxidation number and formal ligand charge; carbonyl ligand, pi-ligands: linear pi systems and cyclic pi systems, complexes containing M-C, M=C and M≡C bonds, hydride and dihydrogen complexes, phosphines and related ligands, spectral analysis and characterization, Dewar-Chat-Duncanson bonding model, isolobal analogy, Agostic interaction

Structure and properties of solids

15 Hours

Crystalline and amorphous solids, lattice, basis, unit cell, symmetry elements, Bravais lattices, close packing in solids (hcp, ccp), voids in close packing, types of bonding in solids, ionic, covalent, metallic, molecular and hydrogen-bonded solids, lattice energy, Born-Haber cycle, Madelung constant, radius ratio rules, crystal field considerations in solids, structure-property correlations. AB and AB₂ type structures, Perovskite structure, Ilmenite structure, Rutile structure, tolerance factor and structural distortion, normal and inverse Spinel structure, cation distribution and magnetic implications, Diamond cubic crystal structure, zinc blende and wurtzite structures, structural comparison and applications. Classification based on SiO₄ tetrahedral linkage, single chain silicates (pyroxenes), double chain silicates (amphiboles), sheet silicates (talc, mica, clay minerals), three-dimensional framework silicates (zeolites), isomorphous substitution, ion exchange properties,

structural chemistry and industrial applications. Point defects, Schottky and Frenkel defects, line defects and dislocations, surface defects and grain boundaries, non-stoichiometric compounds, metal excess and metal deficiency defects, defect equilibria, defect chemistry and its influence on electrical and optical properties, F-center and colorcenters. Free electron theory, band theory of solids, conductors, insulators and semiconductors, intrinsic and extrinsic semiconductors, n-type and p-type semiconductors, superconductivity, critical temperature, Meissner effect, type I and type II superconductors, diamagnetism, paramagnetism, ferromagnetism, antiferromagnetism, ferrimagnetism, cooperative magnetism and magnetic domains. Polarization mechanisms in solids, ferroelectricity, antiferroelectricity, pyroelectricity, piezoelectricity, dielectric properties, liquid crystals (nematic, smectic, cholesteric phases), order parameter and phase transitions, structure–property relationships and technological applications

Reference Books/ Journals

- H. E. White, *Introduction to Atomic Spectra*, McGraw-Hill Kogakusha Ltd, Tokyo, 1934.
- B. N. Figgis, *Introduction to Ligand Field Theory*, Interscience, New York, 1966.
- C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.
- R. McWeeney, *Coulsons' Valence*, 3rd Edn, Oxford University Press, Oxford, 1979.
- A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.
- B. E. Douglas and C. A. Hollingsworth, *Symmetry in Bonding and Spectra, An Introduction*, Academic Press, New York, 1985.
- T. A. Albright, J. K. Burdett and M. H. Whangbo, *Orbital Interactions in Chemistry*, Wiley, New York, 1985.
- V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.
- K. Fukui and H. Fujimoto, *Frontier Orbital and Reaction Paths*, World Scientific, Singapore, 1995.
- J. G. Verkade, *A Pictorial Approach to Molecular Bonding*, 2nd Edn, Springer-Verlag, New York, 1997.
- A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.
- F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley & Sons, Inc, New York, 1999.
- B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley & Sons, Inc., New York, 2001.
- G. Wulfsberg, *Inorganic Chemistry*, Viva Books Pvt Ltd, New Delhi, 2001.
- J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Edn, Pearson, New Delhi, 2006.

- D. A. McQuarrie, P. A. Rock and E. B. Gallogly, *General Chemistry*, 4th Edn, University Science Books, Mill Valley, Canada, 2011.
- A. K. Mukherjee, B. C. Ghosh, *Group theory in Chemistry: Bonding and molecular spectroscopy*, Universities press, 2018
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.
- J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.
- D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University Press, 2001.
- M. Cox, *Optical Properties of Solids*, Oxford University Press, Oxford, 2001.
- G. Aruldas, *Molecular Structure and Spectroscopy*, 2nd Edn, Prentice-Hall of India, New Delhi, 2007.
- C. Trindle and D. Shillady, *Electronic Structure Modeling: Connection between Theory and Software*, CRC Press, Boca Raton, FL, 2008.
- P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry*, 4th Edn, Oxford, 2006. 7
- I. Pelant and J. Valenta, *Luminescence Spectroscopy of Semiconductors*, Oxford, New York, 2012.
- O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
- G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.
- C. N. Satterfield, *Heterogeneous Catalysis in Practice*, McGraw-Hill, New York, 1980.
- P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn, Chapman and Hall, London, 1988.
- J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, VCH, New York, 1997.
- R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 4th Edn, Wiley, New York, 2005.
- C. Elschenbroich, *Organometallics*, 3rd Edn, Wiley-VCH, Weinheim, 2006.
- R. A. van Santen and M. Neurock, *Molecular Heterogeneous Catalysis*, Wiley-VCH, Weinheim, 2006.
- G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, International 2nd Edn, Oxford University Press, Oxford, 2010.
- J. F. Hartwig, *Organotransition Metal Chemistry. From Bonding to Catalysis*, University Science Books, Sausalito, CA, 2010.
- S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, CA, 1993.
- W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, Wiley, New York, 1994.
- I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi, 1998.

- A. Das and G. N. Mukherjee, *Elements of Bioinorganic Chemistry*, 2nd Edn, U. N. Dhur and Sons, Kolkata, 2002.
- A. K. Das, *Bioinorganic Chemistry*, Books & Allied (P) Ltd. Kolkata 2007.
- E. Ochiai, *Bioinorganic Chemistry: A Survey*, Academic Press, Elsevier, 2009.
- R. R. Crichton, *Biological Inorganic Chemistry: A New Introduction to Molecular Structure*, 2nd Edn, Elsevier, New York, 2012.
- R. M. Roat-Malone, *Bioinorganic Chemistry: A short Course*, 2nd Edn, Wiley, New York, 2013.
- G. Patrick, *Instant Notes: Medicinal Chemistry*, Viva Books, New Delhi, 2002.
- G. L. Patrik, *An Introduction to Medicinal Chemistry*, 3rd Edn, Oxford University Press, 2006.
- A. Kar, *Medicinal Chemistry*, 4th Edn, New Age International (P) Ltd, New Delhi, 2007.
- C. G. Wermuth (Ed), *The Practice of Medicinal Chemistry*, Academic Press, Noida, India, 2008.
- D. Sriram and P. Yogeeswari, 2/e, *Medicinal Chemistry*, Pearson
- G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3/e, Pearson.
- A. G. Sharpe, *Inorganic Chemistry*, 3/e, Pearson
- A. F. Hill, *Organotransition Metal Chemistry*, Royal Society of Chemistry, London, 2002.
- A. F. Wells, *Structural Inorganic Chemistry*, 5th Edn, Oxford University Press, Oxford, 1984.
- W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bonds*, Dover Publications, New York, 1989.
- D. M. Adams, *Inorganic Solids*, Wiley, New York, 1992.
- T. C. W. Mak and G. -D. Zhou, *Crystallography in Modern Chemistry*, Wiley, New York, 1992.
- S. R. Elliot, *The Physics and Chemistry of Solids*, John Wiley & Sons, Chichester, 1998. 17
- M. Cox, *Optical Properties of Solids*, Oxford University Press, Oxford, 2001.
- L. E. Smart and E. A. Moore, *Solid State Chemistry: An Introduction*, 4th Edn, CRC Press, Boca Raton, FL, 2012.
- A. R. West, *Solid State Chemistry and Its Application*, 2nd Edn, Wiley-VCH, Weinheim, 2014.

Practical

Credit: 2

Quantitative estimation of pyrolusite (estimation of available oxygen along with other metal ions), dolomite and brass

Reference Books/ Journals

- J. Mendham, R. C. Denney, J. D. Barnes, M. Thomas, *Vogel's Text Book of Quantitative Chemical Analysis* 6th Edition, Pearson Education Asia, Singapore (2002).
- P. Karmakar, S. Ray, R. Sarkar (Sain), A. K. Ghosh, *Concise Practical Chemistry*, New Book Stall, Kolkata (2018).

Chemistry Major/Core CoursePaper Code: **CHEM7012**Paper Title: **Nuclear Analytical General****Credit: 6****Course Objective:**

- The objective is to impart into the students (i) theoretical idea and understanding of nuclear structures and properties, radioactive equilibrium, matter-radiation interaction, statistical methods in analytical chemistry, several thermal methods of analysis, separation techniques, environmental chemistry and cosmochemistry, and (ii) practical knowledge and skills for the estimation of molecular weights, cations and anions, and separation of cations in mixtures by using resins.

Course outcome:

On completion of the course the students will be able to:

- Acquire knowledge on the structure, stability and properties of atomic nucleus along with different disintegration series, their kinetics and activation processes.
- Understand the radioactive radiations, their interaction with matters and related phenomena.
- Realize the radioactivity as a statistical phenomenon and thereby to grasp the importance of statistical methods in the analytical measurement of radioactivity and the related properties.
- Learn and explore different types of methods of elemental analysis, various types of titrations and their applications
- Assimilate ideas on green chemistry and cosmochemistry
- Understand the chemistry behind the separation and estimation of different compounds using ion-exchange resins and thereby acquire skills in designing experiments and/or their need-based extensions.

Theory**Credit: 4****Nuclear properties and structure I****15 Hours**

Liquid drop model, formulation of semi-empirical binding energy equation, mass parabola and application of binding energy equation; nuclear reactions, Q-value and cross section of nuclear reaction, compound nucleus theory (qualitative approach), calculation of fission probability using binding energy equation nuclear angular momentum, magnetic dipole

moment and electronic quadruple moment, parity of nuclear energy states; nuclear size and root mean square radius of atomic nucleus

Radioactive equilibrium 7 Hours

Successive disintegration, Bateman equation, secular and transient equilibrium, no equilibrium; analysis of special types of successive disintegration, formation of radioelement in a nuclear reaction, activation analysis (introductory)

Interaction of radiation with matter 10 Hours

Different radiations, interactions of heavy charged particles, charged particles and photons, energy loss, stopping power and related semi-empirical calculations, Bethe formula, collisional and radiative stopping power, mean excitation energy, range, slowing down time, Cerenkov radiation, attenuation coefficient

Statistical methods in analytical chemistry 7 Hours

Application of counting statistics in analytical and nuclear measurements: probability and binomial distribution, radioactivity as a statistical phenomenon, standard deviation of counting data, Poisson distribution, optimization of counting experiments

Thermal methods 5 Hours

Different methods of analysis: thermogram, TGA, DTA and their applications

Separation techniques 7 Hours

Chromatography: band broadening, column efficiency; column resolution, numerical problems, gas chromatography, high performance chromatography. Ionic liquids: synthesis, properties and applications, green solvent.

Environmental chemistry 4 Hours

Hazardous and Radioactive wastes, treatment, waste management, fertilizer industries

Cosmochemistry 5 Hours

Different geological systems, age of rocks and earth, cosmic rays and its effect in meteorites, comets, black hole, nuclear reactions in stars, solar neutrino hypothesis

Reference Books/ Journals

- B. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice Hall, New York, 1965.
- S. Glasstone, *Source Book of Atomic Energy*, East-West Press Private Ltd, New Delhi, 1967.
- R. D. Evans, *The Atomic Nucleus*, McGraw-Hill, New York, 1979.
- G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, *Nuclear and Radiochemistry*, 3rdEdn, Jhon Wiley & Sons Inc, New York, 1981.
- H. J. Arnikaar, *Essentials of Nuclear Chemistry*, 4thEdn, New Age International (P) Ltd Publications, New Delhi, 2001.
- W. D. Loveland, D. J. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, Wiley Interscience, New Jersey, 2006.
- C. Duval, *Inorganic Thermogravimetric Analysis*, Elsevier Publishing Co, New York, 1963.
- P. Tundo, A. V Perosa and F Zecchimi (Eds), *Methods and Reagents for Green Chemistry: An Introduction*, Wiley Interscience, New Jersey, 2007.
- R. Sanghi and V. Singh, *Green Chemistry for environmental remediation*, Wiley, New York, 2012.
- A. K. De, *Environmental Chemistry*, 4thEdn, New Age International (P) Ltd Publications, New Delhi, 2000.

Practical

Credit: 2

1. Determination of equivalent weight of different salts (NaCl, MgSO₄, ZnSO₄, etc) using cation-exchange resin
2. Determination of the amount of Na⁺ and Mg²⁺ in a mixture using cation-exchange resin
3. Separation and estimation of Zn²⁺ and Mg²⁺ in a mixture by using anion-exchange resin
4. Estimation of chloride ion (Cl⁻) by adsorption and elution over anion-exchange resin

Reference Books/ Journals

- G. H. Jeffery, J. Bassett, J. Mendham, R. C. Denney, *Vogel's Textbook of Quantitative Chemical Analysis* (5th Edition), 1989.
- J. S. Fritz and S. K. Karraker, Ion Exchange Separation of Metal Cations, *Anal. Chem.*, 32, 8, 957–960 (1960).
- Frederick C. Nachod, *Ion Exchange: Theory and Application*, Academic Press, 1940.
- Dr. Inamuddin and Mohammad Luqman, *Ion Exchange Technology II: Applications*, Springer Netherlands, 2014.

Chemistry Major/Core CoursePaper Code: **CHEM7013**Paper Title: **Organic General****Credit: 6****Course Objective:**

- The objective is to impart into the students (i) theoretical idea and understanding of conformation and reactivity of cyclic systems, structure-reactivity relationship, heterocycles, polymers of principles and synthesis, proteins, and (ii) practical knowledge and skills for separation of a binary mixture of liquid-solid/liquid-liquid of organic compounds and identification of functional groups of liquid components

Course outcome:

On completion of the course the students will be able to:

- Learn and accumulate ideas on stereo-chemical conformations and stereo-selective reactivity of various ring systems.
- Understand the structure-activity relationships in quantifying kinetic parameters of aromatic and aliphatic compounds and the role of several factors like conjugation, steric, and solvents, etc. on the parameters.
- Acquire knowledge for the synthesis, reactivity and uses of several heterocycles and their derivatives.
- Understand the classification of proteins, their quality evaluation with some well defined indices, amino acid analysis, and their molar mass determination.
- Grasp the basic ideas of polymers, their structural units, formations and reactions

Theory**Credit: 4****Conformation and reactivity of cyclic systems****15 Hours**

Introduction; reactions on small rings (four and five membered rings); six-membered rings (cyclohexanone, cyclohexene, cyclohexenone, epoxycyclohexane): stereoselectivity in reactions, conformational control in ring formation; Stereoselective reactions of bicyclic compounds: bridged, fused and spiro

Structure-reactivity relationship**8 Hours**

A quantitative approach to Linear free energy relations: Hammett equation, Hammett's σ_x and ρ values and their physical significance through conjugation; deviations from straight line plots; steric effects: Taft equation; solvent effects: Grunwald-Winstein equation

Heterocycles

15 Hours

Synthesis and reactions of 5-membered heterocycle containing two hetero-atoms: imidazole, pyrazole, oxazole, isoxazole, thiazole, isothiazole, triazole and their derivatives

Polymers: principles and synthesis

10 Hours

Monomer, dimer, dendrimer and polymer; mechanism of formation: carbonyl substitution reactions, electrophilic aromatic substitution, the SN^2 reaction and nucleophilic attack on isocyanates; polymerization of alkenes; co-polymerization; biodegradable polymers and plastics; reactions on polymers

Proteins

12 Hours

Classification, evaluation quality: biological value, digestibility co-efficient, PER and NPU; denaturation, structure elucidation; amino acid analysis, molecular weight determinations, tertiary and quaternary structures

Reference Books/ Journals

- D. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn, Wiley Eastern, New Delhi, 1993.
- E. L. Eliel, S.H. Wilen and L.N. Mander, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994.
- R. S. Ward, *Selectivity in Organic Synthesis*, John Wiley & Sons, New York, 1999.
- F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry Part A and Part B*, 4th Edn, Plenum Press, New York, 2001.
- J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.
- J. R. Hanson, *Organic Synthetic Methods*, Royal Society of Chemistry, London, 2002.
- J. H. Fuhrhop and G. Li, *Organic Synthesis, Concepts and Methods*, Wiley-VCH, New York, 2003.
- P. Sykes, *A Guidebook to Mechanism in Organic Chemistry*, 6th Edn, Pearson Education Ltd, New Delhi, 2011.
- R. Kartritzky, *Handbook of Heterocyclic Chemistry*, Pergamon Press, London, 1986.
- R. R. Gupta, M. Kumar, V. Gupta, *Heterocyclic Chemistry II*, Springer Pvt Ltd, India, 2005.
- R. K. Bansal, *Heterocyclic Chemistry*, 4th Edn, New Age International (P) Ltd, India, 2005.
- J. A. Joule, K. Mills, *Heterocyclic Chemistry*, 5th Edn, John Wiley & Sons Ltd, UK, 2010.

K. Nakanishi, T. Goto, S. Ito, S. Natori and S. Nozoe, *Natural Products Chemistry*, Vol I, Academic Press, New York, 1974.

M. P. Stevens, *Polymer Chemistry: An Introduction*, 3rd Edn, Oxford University Press, USA, 1998.

G. R. Newkome, C. N. Moorefield and F. Vogtle, *Dendrimers and Dendron: Concepts, Syntheses, Applications*, Wiley-VCH, Weinheim, 2001.

G. Odian, *Principles of Polymerization*, 4th Edn, Wiley Interscience, New Jersey, 2004.

P. C. Hiemenz and T. P. Lodge, *Polymer Chemistry*, 2nd Edn, CRC Press, Boca Raton, FL, 2007.

Practical

Credit: 2

Separation of following binary mixtures of liquid-solid and liquid-liquid organic compounds by solvent extraction technique and functional group identification of liquid components

Liquid-liquid mixture: aniline + diethyl malonate, aniline + ethyl benzoate, aniline + benzyl alcohol, m-toluidine + cyclohexanol, m-anisidine + cyclohexanol

Liquid-solid mixture: benzyl alcohol + p-nitrobenzoic acid, aniline + benzanilide, diethyl malonate + p-nitrophenol, acetophenone + salicylic acid, cyclohexanol + p-nitroaniline

Reference Books/ Journals

A. I. Vogel, *Elementary Practical Organic Chemistry: Qualitative Organic Analysis Part 2*, CBS Publishers and Distributors

Chemistry Major/Core Course

Paper Code: **CHEM7014**

Paper Title: **Physical General**

Credit: 6

Course Objective:

- The objective is to impart into the students (i) theoretical idea and understanding on symmetry and group theory with applications, fundamentals quantum mechanics, theories and applications of chemical kinetics, electrochemistry; thermodynamics and statistical mechanics, and (ii) practical knowledge and understanding of the experiments on kinetics and equilibrium and develop skills in handling instruments (like, conductivity-bridge, potentiometer, colorimeter, polarimeter, etc.)

Course outcome:

On completion of the course the students will be able to:

- Learn and identify the symmetry elements and operations and hence the point group of an object including fullerene, construct representations and hence character table of a point group and use it in analyzing and solving physicochemical problems
- Get hold of projection operator and hence its use in calculating SALCs and MOs under Hückel approximations for some simple system
- Analyze the quantum mechanical postulates, understand conversion of orthonormal functions from degenerate functions, Heisenberg uncertainty principle and its consequences
- Understand quantum mechanical equation of motion and related theorems and handle several exactly solvable problems, like step potential and tunnelling, the Virial theorem, harmonic oscillator, rigid rotator, Dirac delta function, Fourier Transform, etc.
- Get the ideas behind the theories of reaction rate and thereby derive the corresponding rate expressions.
- Apply the theories in thermodynamic formation of reaction rates in studying uni-, bi- and ter-molecular reaction rates, and other consequences thereof.
- Understand statistical interpretation of thermodynamics, express thermodynamic functions, specific heats of solids, and equilibrium constant of a reaction in terms of partition functions and interpret equipartition principle.
- Realize ion-solvent interaction in reference with several models and hence calculate the change of thermodynamic parameters, solvation number, ion-association, ion association constant, factors responsible for.
- Understand concept of electrode kinetics relating current with rates of electrode reactions and hydrogen electrode with its application in charge transfer reaction.

Theory**Credit: 4****Symmetry and group theory****15 Hours**

Point symmetry operations, groups and group multiplication tables, similarity transformation and conjugate classes, identification of point groups and stereographic projection, symmetry elements and symmetry operations of the Platonic solids, symmetry of the fullerene [60] structure; representation of symmetry operators and groups; characters of symmetry operators in a representation, invariance of character under similarity transformation, rules (without derivation) for construction of character tables with illustrations

The Great Orthogonality Theorem: statement and interpretation, proof of important corollaries; construction of character tables, cyclic groups and construction of their character tables, direct product groups, direct product representations, projection operators (without derivations) and vanishing of integrals, invariance of the Hamiltonian operator and eigenfunctions of Hamiltonian operator (H) as bases of irreducible representations, SALCs and their use in calculating π MOs under the Hückel approximations for some simple systems, outlines of symmetry aspects of molecular spectra

Quantum mechanics III

12 Hours

Analysis of quantum mechanical postulates - pictures and representations; properties of sets of functions, operators and related theorems; degeneracy, spread of observation and uncertainty principle; Schmidt orthonormalisation; Fourier transformation, delta function with examples, free particle normalization, matrix formulation, bound states, the Virial theorem

Equation of motion, constants of motion; Ehrenfest's theorem, exactly solvable problems: step potential and tunneling, bound states, the Virial theorem, harmonic oscillator, rigid rotator; elementary discussion of the H-atom solution

Chemical kinetics III

13 Hours

Theories of reaction rates: applications to uni-, bi- and termolecular reactions, thermodynamic formulation of reaction rate, reactions in solution cage effect, diffusion and activation controlled reactions (elementary idea), dielectric effect on ion-ion reaction, electrostriction, volume of activation, effect of pressure on reaction rate, classification of reactions on the basis of volume of activation, study of fast reactions flow process and relaxation techniques; Curtin-Hammett principle, linear free energy relationship, Hammett and Taft equations

Electrochemistry III

10 Hours

Introduction, ion-solvent interaction: Born model and Born equation, enthalpy, entropy and free energy of ion-solvent interaction and their calculations, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant, factors responsible for ion association; effect of ion association over conductivity; ion-dipole and ion-quadrupole interactions; electrode kinetics: relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation and its importance; Hydrogen electrode and its application in charge transfer reaction.

Statistical Thermodynamics II

10 Hours

Legendre transformation with applications; Maxwell-Boltzmann distribution with degeneracy (for both distinguishable and indistinguishable particles), partition function and its properties, interpretation of thermodynamic laws, thermodynamic function in terms of partition functions,

molecular partition functions (translational, rotational, vibrational and electronic) for ideal gas, calculation of thermodynamic functions for monoatomic and diatomic gases, equipartition principle, equilibrium constant, theories of specific heat of solids

Reference Books/ Journals

- S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.
- V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.
- D. M. Bishop, *Group Theory and Chemistry*, Oxford University Press, 1993.
- A. K. Mukherjee and B. C. Ghosh, *Group Theory in Chemistry: Bonding and Molecular Spectroscopy*, Universities Press (India) Private Ltd., Hyderabad, 2018
- A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3rdEdn, John Wiley & Sons, New York, 1999.
- L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
- I. N. Levine, *Quantum Chemistry*, Pearson, New York, 2014.
- P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
- L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.
- A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
- F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.
- D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt Ltd, New Delhi, 2003.
- S. Glasstone, *An Introduction to Electrochemistry*, D. Van Nostrand Company, 1962.
- J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol I, Plenum Press, New York, 1970.
- I. N. Levine, *Physical Chemistry*, Tata McGraw-Hill, New Delhi, 1978.
- K. J. Laidler, *Reaction Kinetics*, Vols I and II, Pergamon Press, London, 1970.
- L. P. Hammett, *Physical Organic Chemistry*, McGraw-Hill Book Company, New Delhi, 1970.
- J. Albery, *Electrode Kinetics*, Oxford Chemistry Series, Clarendron Press, Oxford, 1975.
- K. J. Laidler, *Chemical Kinetics*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988.
- M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, 1999.
- K. Denbigh, *Principles of Chemical Equilibrium*, Cambridge University Press, Cambridge, 1981.
- I. M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, John Wiley, New York, 1994.
- G. W. Castellan, *Physical Chemistry*, 3rdEdn, Narosa Publishing House, 1995.
- N. A. Gokcen and R. G. Reddy, *Thermodynamics*, Plenum Press, New York, 1996.
- G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall, India, 1997.

P. W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.

R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.

D. A. McQuarrie and J. D. Simon, *Molecular Thermodynamics*, University Science Books, California, 1999.

Practical

Credit: 2

1. Experiments on kinetics:

- (a) Decomposition H_2O_2 by FeCl_3
- (b) Reaction between $\text{K}_2\text{S}_2\text{O}_8$ and KI analytically and/ or spectrophotometrically
- (c) Activation energy of clock reaction
- (d) Inversion kinetics of cane sugar (polarimetrically)

2. Experiments on equilibrium:

- (a) Conductometric and potentiometric titrations of (i) weak acid and (ii) mixtures of weak acids and bases for determination of pK_a values of the concerned acid(s)
- (b) Potentiometric titration of AgNO_3 solution by KCl solution for the determination of K_{sp} of AgCl
- (c) Hydrolysis constant (K_h) of aniline hydrochloride by conductometric method
- (d) Ternary phase diagram for (water-chloroform-acetic acid) system
- (e) Coordination number of copper in cuproammonium complex by partition method

Reference Books/ Journals

P. B. Levitt, *Findlays Practical Physical Chemistry*, Longman's London (1966).

D. Shoemaker and C. Garland, *Experiments in Physical Chemistry*, McGraw Hill International Edition (1966).

H. W. Salberg J. I. Morrow, S. R. Cohen and M. E. Green, *Physical Chemistry Laboratory Principles and Experiments*, Macmillan publishing Co., New York (1978)

D. Farrington, *Experimental Physical Chemistry*, McGraw Hill, New York (1956).

A.M James and P. E. Pritchard, *Practical Physical Chemistry*, Longman's Group Ltd. (1968).

J. M. Wilson, R. J. Newcombe, A. R. Denaro and R. M. W. Rickett, *Experimental Physical Chemistry*, Pergamon Press, New York (1962).

J. C. Ghosh, *Experiments in Physical Chemistry*, Bharati Bhawan (P & D), Patna (1988).

J. B. Yadav, *Advanced Practical Physical Chemistry*, Goel Publishers, Meerut (1988).

B. C. Kosla, *Senior Practical Physical Chemistry*, Simla Printers, New Delhi (1987).

R.C. Behra & B Behra, *Experimental Physical Chemistry*, Tata McGraw, ND (1983)

V. D. Atavale and Parul Mathur, Experimental Physical Chemistry, New Age International, New York (2001).

Chemistry Minor Course

Paper Code: **CHEM7021**

Paper Title: **Industrial Chemistry**

Credit: 4

Course Objective:

- The objective is to impart into the students the theoretical idea and understanding on classification and characteristics of fuels and combustion, macromolecular polymers, glass with classification and structures, spectroscopic techniques like, UV–Visible, atomic absorption, fluorescence and mass spectrometry, and analytical data analysis

Course outcome:

On completion of the course the students will be able to:

- Grasp the general ideas on various kinds of fuels, their combustion, calorific values, etc.
- Learn and understand polymers, their preparations, characteristics, average molar masses and different methods of determinations, etc.
- Acquire knowledge on glass and ceramics, methods of fabrication of different wares, porcelain and vitreous enamels, etc.
- Develop understanding on various analytical tools, techniques and analysis of data obtained from instruments like, UV-Vis., IR, AAS, Fluorescence, NMR, Mass spectroscopy.

Theory

Credit: 4

Fuels and combustion

14 Hours

classification of fuels, characteristics of good fuel, combustion reactions, air requirement, calorific value, bomb calorimeter, Dulong's formula, solid fuels, coal, coke, carbonization, proximate analysis, ultimate analysis, liquid fuels, petroleum, refining, fractional distillation, cracking, octane number, cetane number, synthetic petrol, gaseous fuels, natural gas, LPG, CNG, producer gas, water gas, petrochemicals,

feedstocks, olefins, aromatics, nuclear fuels, fission, fusion, uranium, thorium, nuclear reactor, bio-fuels, bioethanol, biodiesel, biogas, transesterification

Macromolecular Polymers

14 Hours

Classification, polymerization - addition polymerization, condensation polymerization, ring opening, etc., polymerization techniques; degree and extent of polymerization, molecular weights and its determination- osmometry, viscometry, light scattering, sedimentation, thermoplastics, thermosetting polymers, elastomers, fibers, biopolymers, conducting polymers, polymer characterization, glass transition temperature, thermal analysis, mechanical properties, industrial polymers

Glass

6 Hours

Classification and structure, soda-lime glass, borosilicate glass, lead glass, manufacture, clays, kaolin, ball clay, fire clay, silica, ceramics, slip casting, dry pressing, isostatic pressing, sintering, porcelain, vitreous enamels

Spectroscopic techniques

20 Hours

UV-Visible spectroscopy: Beer–Lambert law, electronic transitions, instrumentation

IR spectroscopy: Molecular vibrations: functional group analysis

Atomic absorption spectroscopy: Flame method, graphite furnace

Fluorescence spectroscopy: Fluorescence, phosphorescence, nuclear magnetic resonance, chemical shift, spin–spin coupling

Mass spectrometry: Ionization methods, mass analyzer, fragmentation

Analytical data analysis

6 Hours

Calibration curve, accuracy, precision, standard deviation, limit of detection, limit of quantification, error analysis

Reference Books/ Journals

J. Griswold, Fuels, combustion and furnaces, McGraw-Hill Book Company, Inc., London (1946).

J R. Puskar, Fuel and Combustion Systems Safety, John Wiley & Sons, Inc. (2014).

S. Sarkar, FUELS AND COMBUSTION (3/E), Universities Press (2009).

O.P. Gupta, Elements of Fuel & Combustion Technology, Khanna Book Publishing Company (P) Ltd., New Delhi (2018).

C. Tanford, *Physical Chemistry of Macromolecules*, John Wiley & Sons, Inc, New York, 1961.

F. W. Billmeyer, *Text Book of Polymer Science*, 2ndEdn, Wiley-Interscience, New York, 1971.

G. S. Mishra, *Introductory Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.

- P. Ghosh, *Polymer Science and Technology of Plastic and Rubber*, Tata McGraw-Hill Publishing Company Limited, New Delhi, 1993.
- S. F. Sun, *Physical Chemistry of Macromolecules: Basic Principles and Issues*, John Wiley & Sons, New York, 1994.
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- I. N. Levine, *Physical Chemistry*, 4thEdn, Tata McGraw-Hill, New Delhi, 1995.
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- D. A. Skoog, D. M. West, F. J. Holler and S. R. Crouch, *Fundamentals of analytical chemistry* 9/E, Brooks/Cole Pub Co. (2003).
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- R. K. Das, *Industrial chemistry*, Asia Publishing House (1967).
- S.M. Rao, A.B. Majali, R.G. Deshpande, T.S. Murthy (eds.), *Industrial Applications of Radioisotopes and Radiation. A record of the contributions at the International Conference on Applications of Radioisotopes and Radiation in Industrial Development (March 1-3, 1984 Bombay, India)*, John Wiley & Sons Inc. (1986).

SEMESTER VIII

(Hons. with Research Project/ Dissertation)