CHEMISTY

PG- MSc. Syllabus

Code	Name of Paper	Credits	Marks
1st Semester			
CHE-PG-C101	Chemistry I	4	100
CHE-PG-C102	Chemistry II	4	100
CHE-PG-C103	Mathematics and Biochemistry	4	100
CHE-PG-C104	Practicals I	4	100
2nd Semester			
CHE-PG-C201	Inorganic Chemistry	4	100
CHE-PG-C202	Organic Chemistry	4	100
CHE-PG-O203	Physical Chemistry	4	100
CHE-PG-C204	Practicals II	4	100
3rd Semester			
CHE-PG-O301	Instrumental Techniques	4	100
CHE-PG-E3XY	Elective I	4	100
CHE-PG-E3XY	Elective II	4	100
CHE-PG-C304	Practicals III	4	100
4th Semester			
CHE-PG-E4XY	Elective III	4	100
CHE-PG-E4XY	Elective IV	4	100
CHE-PG-E4XY	Elective Practical	4	100
CHE-PG-E404	Project	4	100
TOTAL		**36**	**1600**

Semester I

CHE-PG-C101: Chemistry I 4 credits

Unit I: Stereochemistry and bonding in Main group compounds

Valence Shell Electron Pair Repulsion model, stereochemical rules and explanation of the shapes of molecules and ions of non-transition elements with 2-7 valence shell electron pairs. Walsh Diagram. Bent rule and energetics of hybridization.

HSAB: Classification of acids and bases as hard and soft; HSAB principle, theoretical basis of hardness and softness; Lewis-acid base reactivity approximation; Group Characteristic of Lewis Acids & Base (group 13, 14, 15, 16, 17 and s-block) donor and acceptor numbers, E and C equation; applications of HSAB concept.

Unit II: Group Theory and Symmetry of molecules

Group Theory: Definition of group, symmetry, point groups, representation of group, Abelian group, Group multiplication table, Groups, sub-groups and classes, Symmetry operations and symmetry elements, Point group, classification and symmetry number, Schoenflies symbols. orthogonality theorem, irreducible representation, character table, Point group symmetry and optical activity, dipole moment, vibrational spectroscopy and bonding.

Unit III: Aromaticity

Benzenoid and nonbenzenoid systems, antiaromaticity and non aromatic compounds.

Effects of Structure on Reactivity: Hammett equation, Linear free energy relationships (LFER) and substituent and reaction constants. Structure-activity relationship. Taft equation.

Aliphatic Nucleophilic Substitution at Saturated Carbon: Mechanism and Stereo-chemistry of S_N1, S_N2, S_Ni, S_N1' and S_N2' reactions. Neighboring group participation. Classical and non-classical carbocations. The reactivity effects of substrate structure, solvent effects, competition between S_N1 and S_N2 mechanisms. Phase transfer catalysis, ambident nucleophilicity, regioselectivity.

Aromatic Electrophilic Substitution: The Arenium ion mechanism, orientation and reactivity in monosubstituted benzene rings, ortho/ para ratio. Ipso substitution. Effect of substrates, leaving groups and solvent polarity on the reaction.

Aromatic Nucleophilic substitution: Aromatic S_NAr, S_N1, S_N2 and benzyne mechanisms. Reactivtiy : effect of substrate structure, leaving group, and attacking nucleophile

Unit IV: Addition to Carbon–Carbon Multiple Bonds

Electrophilic, free-radical and nucleophilic mechanisms-Mechanistic and Stereochemical aspects. Orientation and reactivity. Hydroboration and Michael reaction.

Elimination reactions: The E1, E2 and E1cB mechanisms, Orientation of the double bond. Hofmann versus Saytzeff elimination, Pyrolytic syn-elimination- Chugaev and Cope eliminations, Competition between substitution and elimination reactions.

Nucleophilic Addition to Carbonyl Compounds

Hard and soft nucleophiles, addition to conjugated carbonyls; Competition between 1,2 and 1,4 addition, Meerwin-Pondorf Reaction, Cannizaro reaction, stetter reaction, Aldol condensation, Grignard reagent, alkyl lithium, Perkin reaction, Benzoin condensation, Benzilic acid rearrangement, Wittig reaction,

References

1. Cotton, F.A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons, New York.
2. Huheey, J. E., 1993 Inorganic Chemistry, 4th Ed., Addison-Wesley Pub. Co., New York.
3. Drago, R. S., 1971 Physical Methods in Inorganic Chemistry, International Edn., Affiliated East-West Press, New Delhi.
4. Shriver, D. F. and Atkins, P. W., 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
5. Cotton, F. A., Wilkinson, G. and Gaus, P.L., Basic Inorganic Chemistry, 3rd Edition, John Wiley & Sons, New York.
6. Greenhood, 1976, Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
7. Lee, J. D. 1999 Concise Inorganic Chemistry, Blackwell Science.
8. Purcell K. F. and Kotz J. C., 1987 Inorganic Chemistry, W. B. Sauders Com. , Hong Kong.
9. Cotton, F.A. 1990 Chemical Application of Group Theory, 3rd Ed, Wiley-Blackwell.
10. Smith M. B. and March, J. 2001 March's Advanced Organic Chemistry, 6th Edn, John Wiley & Sons, New York.
11. Sykes, P. 1997 A Guide book to Mechanism in Organic Chemistry, 6th Edition, Orient Longman Ltd., New Delhi.
12. Fryhle, S. Organic Chemistry, 8th Edition, John Wiley & Sons, New York.
13. Clayden, J., Greeves, N. , Warren, S. and Wothers, P., 2000 Organic chemistry, Oxford University Press.
14. Bruice, Organic Chemistry, 5th Edition, Pearson Education
15. Carey F. A. and Sundburg R. J. 2007 Advance Organic Chemistry; 5th Ed. Springer
16. Mukherjee S. M. and Singh, S. P, 1990 Reaction Mechanism in Organic Chemistry, Ist Edition, Macmillan India Ltd., New Delhi.
17. Lowry T.H. and Richardson, K. S. 1998 Mechanism and Theory in Organic Chemistry, 3rd Edition, Addison – Wesley Longman Inc. (IS Edition)
18. Morrison R. T. and Boyd, R. N. 2003 Organic Chemistry, 6th Edition, Prentice- Hall of India, New Delhi.
19. Kalsi, P. S. 1996 Organic Reactions and Their Mechanisms, Ist Edition, New Age International Publication, New Delhi.

CHE-PG-C102: Chemistry II 4 credits

Unit I: Metal-Ligand Bonding in Transition Metal Complexes

Crystal field splitting diagrams in complexes of low symmetry; Spectrochemical and Nephelauxetic series; thermodynamic and structural effects; site selection in spinels, Jahn-Teller distortions; experimental evidence for metal-ligand orbital overlap; ligand field theory, molecular orbital theory of octahedral complexes, brief introduction to Angular Overlap Model. Electronic spectra of Transition Metal Complexes: Spectroscopic ground states; Orgel energy level and Tanabe-Sugano diagrams for transition metal complexes; Charge transfer spectra; electronic spectra of octahedral and tetrahedral Co(II) and Ni(II) complexes and calculation of ligand-field parameters. Russell-Saunders coupling for d^n states. Splitting of one-electron levels in an octahedral environment. Correlation diagram. The method of descending symmetry, selection rules. Spectral transition probability, vibronic coupling, non-centrosymmetric complexes, polarization of allowed transitions.

Unit II: Thermodynamics

Review of Laws of Thermodynamics. Entropy, free energy and chemical potential. Partial molar properties and their significance. Fugacity: its concept and determination. Properties of ideal solutions; non-ideal systems-deviations (negative and positive) from ideal behaviour, excess functions for non-ideal solutions, calculations of partial molar quantities, determination of partial molar volume and partial molar enthalpy.

Non equilibrium Thermodynamics Thermodynamic criteria for non-equilibrium process, Entropy production and entropy flow, Entropy balance equations for heat flow, chemical reactions etc., Transformations of the generalized fluxes and forces, Nonequilibrium stationary states, Generalized flux and forces, Phenomenological equations, Onsager reciprocal relations, Principle of detailed balance, Electro kinetic phenomenon, Diffusion, Electric conduction, Transport number and electrochemical cells, Irreversible thermodynamicc for biological systems

Unit III: Electrochemistry

Theory of electrolytes, Ion-electron theory; Debye Huckel Limiting law, Activity Coefficients, Metal/Electrolyte interface: Outer Helmholtz Potential (OHP) and Inner Helmholtz Potential (IHP), potential profile across double layer region, potential difference across electrified interface; Structure of the double layer: Helmholtz-Perrin, Gouy-Chapman (Poisson-Boltzmann equation), and Stern models. Butler-Volmer equation under near equilibrium and non- equilibrium conditions, exchange current density, Tafel plot. Polarizable and non-polarizable interfaces. Electrochemical cells and Batteries.

Unit IV:

Micelles and Macromolecules: Surface active agents and their classification, micellization, hydrophobic interaction, critical micellar concentration (cmc), factors affecting cmc of surfactants, counter ion binding to micelles, thermodynamics of micellization-phase separation and mass action models, solubilization, micro emulsions, reverse micelles. Polymers-definition, types of polymers, liquid crystal polymers. Molecular mass-number and mass average molecular mass, determination of molecular mass (osmometry, viscosity, light scattering methods, Gel Permeation chromatography).

Colloids: Multimolecular, macromolecular and associated colloids. Stability of collids. The zeta potential. Kinetic, optical and electrical properties of colloids. Electrokinetic phenomena: Electrophoresis, electroosmosis, sedimentation potential and streaming potential. Donnan membrane equilibrium. Collodal quntum dots, Metal nanoparticles and magnetic nanoparticles. Size dependent optical and electrical properties. Supermagnetic limit

References

1. Cotton, F.A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons, New York.
2. Huheey, J. E., 1993 Inorganic Chemistry, 4th Ed., Addison-Wesley Pub. Co., New York.
3. Drago, R. S., 1971 Physical Methods in Inorganic Chemistry, International Edn., Affiliated East-West Press, New Delhi.
4. Shriver, D. F. and Atkins, P. W., 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
5. Cotton, F. A., Wilkinson, G. and Gaus, P.L., Basic Inorganic Chemistry, 3rd Edition, John Wiley & Sons, New York.
6. Greenhood, 1976, Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
7. Lee, J. D. 1999 Concise Inorganic Chemistry, Blackwell Science.
8. Purcell K. F. and Kotz J. C., 1987 Inorganic Chemistry, W. B. Sauders Com. , Hong Kong.
9. Cotton, F.A. 1990 Chemical Application of Group Theory, 3rd Ed, Wiley-Blackwell.
10. Bockris J.O'M., and Reddy, A. K. N. 1998 Modern Electrochemistry, Vol. 1 & Vol. 2 AB, Second Edition, Plenum Press, New York.
11. Castellan G. W., Physical Chemistry, Addison-Wesley Publishing Company, Reading, MA.
12. Atkins, P. W. , 2002 Physical Chemistry, Seventh Edition, Oxford University Press, New York.
13. Levine, I. N. 2002 Physical Chemistry, 5th Edition, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
14. Ram J. Raja and Kuriacose, J.C. 1993 Kinetics and Mechanism of Chemical Transformations, MacMillan Indian Ltd., New Delhi.
15. Barrow, G.M. Physical chemistry, 3rd edn., international student edition, McGraw-Hill
16. Glasstone. S. 1940, Text - book of physical 1940. Publisher: Van Nostrand.
17. Pilling M. J. and Seakins, P. W. 1995 Reaction Kinetics, Oxford University Press, 1995
18. Moore, W. J. 1972, Physical Chemistry, Prentice Hall College Div; 4th edition
19. Engel T. and Reid P., Physical Chemistry, Pearson Education

CHE-PG-C103: Mathematics and Biochemistry 4 credits

Unit I: Functions: Linear, Quadratic, Cubic, Logarithmic, Exponential, Trigonometric, Hyperbolic.

Differential and integral calculus, limits, derivative, physical significance, basic rules of differentiation, maxima and minima, applications in chemistry, exact and inexact differential, periodic function, Taylor and McLaurin series, curve sketching, partial differentiation, rules of integration, definite and indefinite integrals..

Differential equations Separation of variables, homogeneous, exact, linear equations, equations of second order, series solution method. Fourier series and analysis. Complex numbers. Laplace transformation.

Unit II: Permutations, combinations and theory of probability distributions Binomial, Gaussian and Poisson. 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. Complex Variables

Unit III: Carbohydrates: Glycosides, Oligosaccharides and polysaccharides. Role of sugar in molecular recognition. Nucleic Acids: RNA, DNA, base-pairing, double helical structure of DNA, Gene regulatory protein- Zinc finger protein.
Aminoacids and Proteins: Aminoacids, peptide links and oligopeptides. Proteins: primary, secondary, tertiary, and quaternary structure of proteins. Structure, purification and denaturation of proteins.
Lipids and membranes: Lipids, fatty acids, Classification of lipids, self-association of lipids-micelles, reverse micelles and membranes, transport of cations through membranes.

Unit IV: Metabolism and Energetics

Catabolic and anabolic processes, glycolysis, citric acid cycle and oxidative phosphorylation. Photosystems (PSI & PSII).

Enzyme Enzyme kinetics and applications of enzymes in organic synthesis. Enzyme inhibitors and co-enzymes in organics reactions. Drugs based on enzyme inhibition.

Metal ions in biological systems and their role in ion transport across the membranes (molecular mechanism) Oxygen-uptake proteins, cytochromes and ferredoxins. Oxygen uptake proteins: Hemoglobin, Myoglobin, hemerythrin and hemocyanin. Metal complexes in medicine. Chemotherapy.

References

1. Mortimer R. G., Mathematics for Physical Chemistry, Elsevier.
2. Steiner E. 1996The Chemical Maths Book, , Oxford University Press.
3. Daniels F. , 1972 Mathematical Preparation for Physical Chemistry, , McGraw Hill
4. Margenau, H and Murphy , G. M. 1956 The Mathematics of Chemistry and Physics- van Nostrand, Princeton, NJ.

5. Norris A. C. Computational Chemistry, John Wiley
6. Press, W. H. , Teukolsky, S. A. Vetterling, W. T. and Flannery B. P. 1996 Numerical Recipes in FORTRAN/C by, Cambridge University Press, 2nd Ed.
7. Xavier , C. 2002 Fortran 77 and Numerical Methods b, New Age International,
8. Boas, M. L. Mathematical Methods in the Physical Sciences, Wiley; 2nd edition.
9. Stryer L., 2002 Biochemistry, 5th edition, Freeman & Co., New York.
10. Nelson D. L. and Cox M.M., 2002 Lehninger Principles of Biochemistry, 3rd edition McMillan North Publication.
11. Hughes M. N. , 1981 Inorganic Chemistry of Biological Processes, John Wiley.
12. Smith M.B., 1995 Organic Synthesis, McGraw Hill Inc., New York.
13. Ariga K. and Kunitake T. 2006 Supramolecular Chemistry – Fundamentals and Applications, Springer
14. Crabtree R. H., Organometallics in Organic synthesis Vol-II – Organometallics of Transition Metals in Organic Synthesis
15. Voet D., Voet J.G and Pratt C. W., 1999 Fundamentals of Biochemistry, John Wiley & Sons, New York

CHE-PG-C104: Practicals I 4 credits

Inorganic Chemistry Experiments

A. Ore Alloy and Commercial Product Analysis: (Any two)

A.1. Determination of Silica and Manganese in pyrolusite

1. Determination of Copper and iron from chalcopyrite.
2. Determination of iron from hematite by complexometric titration.
3. Determination of tin & lead from solder.
4. Determination of iron & chromium from mild steel.
5. Determination of copper and nickel from cupronickel.
6. Determination of iron from hematite using UV-Vis spectrophotometer.
7. Determination of phosphoric acid in soft drinks
8. Analysis of Cement
9. Determination of Flouride in toothpaste.

B. Preparation and Characterization of the following compounds (Any seven preparations are to be completed):

B.1. Tris (oxalate) manganese (III)
B.2. Tetrapyridinesilver (II) peroxidisulphate
B.3. Tris (acetylacetonato) iron (III)
B.4. Bis (N,N-diethyldithiocarbamato) nitrosyliron (I)
B.5. Optical isomers of tris (ethylenediamine) cobalt (III) chloride
B.6. Linkage isomers of nitro and nitritopentamminecobalt (III) chloride
B.7. Ferrocene or dibenzene chromium
B.8. Hydridochlorocarbonyl tris (triphenylphosphine) ruthenium (II)
B.9. Tris(2,2'-bipyridine)ruthenium (II) perchlorate
B.10. $[(p\text{-(cymene)}RuCl_2]_2$
B.11. Tris (acetylacetonato) manganese (III)
B.12. Copper(I) Thiourea complexes: $[Cu(Tu)_6]SO_4 . H_2O$

Characterization includes microanalysis, magnetic susceptibility and conductance measurements and infrared, UV-Visible, NMR spectroscopy, XRD and cyclic voltammetry studies.

Books Recommended:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. A text book of Quantitative Inorganic Analysis – A. I. Vogel
3. Experimental Inorganic Chemistry - W. G. Palmer
4. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.
5. Chemistry experiments for Instrumental Methods by Donald T. Sawyer, William R. Heineman & Jalice M. Beebe , John Wiley & Sons ,1984.
6. Experimental Physical Chemistry by G. Peter Matthews, Clarendon Press, 1985.
7. Modern Experiments for Introductory Chemistry, compiled by Neidig and Strattom, 2nd Ed., Reprinted from Journal of Chemical Education,1990.
8. Handbook of Inorganic Synthesis: G. Brauer
9. Inorganic Synthesis: R. B. King
10. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, GregoryGirolami, Thomas B. Rauchfuss and Robert J. Angelici. University Science Books.

Semester II

CHE-PG-C201: Inorganic Chemistry 4 credits

Unit I: Chemistry of non-transition elements: Non-transition metal chemistry. Synthesis, Properties, Structure and Bonding: Nitrogen, Phosphorous, Sulfur, Pseudohalogen, Interhalogen and Xenon Compounds; Boranes, Carboranes, Metallocarboranes, Borazines, Phosphazenes, Sulfur-Nitrogen compounds, silicates, silicones.

Isopoly and Heteropoly Acids and Salts

Synthesis, structural principles and application of V, Nb, Ta, Cr, Mo and W polyacids

Unit II: Kinetics and Mechanism of transition metal complexes

Energy profile of reactions, discussion on general reactivity of metal complexes, inert and labile complexes, different types of mechanisms (D, A, I_a and I_d). Techniques for experimental measurements of reaction rates, techniques for fast reaction. Substitution reactions: Application of CFT, mechanism of ligand substitution in octahedral complexes, mechanism of isomerization and racemization, Twist mechanism of racemization, substitution reactions in square planar complexes. Cis- and trans- effects.

Unit III: Electron Transfer Reactions: Mechanism of redox reactions with reference to metal complexes. Electron transfer reactions – outer sphere and inner sphere, atom transfer, induced electron transfer reactions, two electron transfer reactions, non complementary reactions, synthetic implications of electron transfer reactions, solid state electron transfer reactions. Electroprotic reactions, Marcus-Husch theory, correlation between thermal and optical electron transfer reactions; identification of intervalence transfer bands in solution

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Unit IV: Metal Carbonyls

Metal carbonyls: Synthesis, structure and reactivity; bonding in metal carbonyls, variants of CO bridging, vibrational spectra of metal carbonyls, principal reaction types of metal carbonyls. Low nuclearity (M3-M4) and high nuclearity (M5-M10) carbonyl clusters. Metal-metal bonding(MO), skeletal electron counting. Wade-Mingos Lauher rule, isolobal analogy. Halide clusters of Nb, Ta, Mo, W, Re. Synthesis, structure and bonding. Interstitial Clusters-hydrides, carbides and nitrides.

References:

1. Huheey, J. 1993 E. Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York.
2. Cotton F. A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John- Wiley & Sons, New York.
3. Crabtree, R.H. 1988 The Organometallic Chemistry of the Transition Metals, 1st Edn., John-Wiley & Sons, New York.
4. Shriver , D. F. and Atkins, P. W. 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
5. Greenhood, 1976 Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
6. Cleydon, J. , Greeves, N. , Warren, S. and Wolthers, P. , 2001 Organic Chemistry: Oxford
7. Collman, J. P. , Hegedus, L. S. , Norton J. R and Finke, Richard G. 1987 Principles and Applications of Organotransition Metal Chemistry, 1st Edn., University Science Books, Mill Valley, California.
8. Elschenbroich, Ch. and. Salzer, A, 1991 Organometallics: A Cosize Introduction, 2nd Edn.,VCH

CHE-PG-C202: Organic Chemistry 4 credits

Unit I: Pericyclic Reactions

Molecular orbital symmetry, Frontier orbitals of ethylene, 1,3-butadiene, 1,3,5-hexatriene and allyl system. Classification of pericyclic reactions. Woodward-Hoffmann correlation diagrams. FMO and PMO approach. Electrocyclic reaction; conrotatory and disrotatory motions 4n, 4n+2 and allyl systems. Cycloaddition; antrafacial and suprafacial addition, 4n and 4n+2 systems, 2+2 addition of ketenes, 1,3 dipolar cycloadditions and cheleotropic reactions. Sigmatropic Rearrangements; suprafacial and antrafacial shifts of H, sigmatropic shifts involving carbon moieties, 3,3- and 5,5- sigmatropic rearrangements, Claisen, Cope and Aza-Cope rearrangements. Ene reaction.

Unit II: Reagents in Organic Synthesis

Use of the following reagents in organic synthesis and functional group transformations; complex metal hydrides, Gilman's reagent, lithium dimethylcuprate, lithium diisopropylamide (LDA), dicyclohexylcarbodiimide, 1,3-dithiane (reactivity Umpoloung), trimethylsilyl iodide, tri-n-butyltin hydride, Woodward and pervost hydroxylation, osmium tetroxide, DDQ, selenium

dioxide, Phase transfer catalysts, crown ethers and Merrifield resin, Peterson's synthesis, Wilkinson's catalyst, Baker yeast.

Unit III: Heterocyclic Chemistry

Synthesis and reactivity of furan, thiophene, pyrrole, pyridine, quinoline, isoquinoline and indole; Skraup synthesis, Fisher indole synthesis.
Chemistry of Natural Products: Structure elucidation and biosyntheses of Alkaliods, Terpenoids, Steroids.

Unit IV: Esterification, Hydrolysis of Esters and Photo Chemistry

Evidence for tetrahedral intermediate in BAc^2 and AAc^2 mechanisms, steric and electronic effects. The AAc^1 and other pathways involving alkylto-oxygen bond cleavage.

Introduction to various reactions in Photochemistry.

References

1. Fleming, I. 1976 Frontier Orbital and Organic Chemical Reactions John Wiley,.
2. Carruthers, W. 1990 Some modern Methods of Organic Synthesis Cambridge University Press.
3. Greene, T.W. 1999 Protective Groups in Organic Synthesis Wiley-VCH,.
4. Smith M.B. and March, J. 2001 March's Advanced Organic Chemistry, 5th Edition, John Wiley & Sons, New York.
5. Joule J. A. and Mills, K. Heterocyclic Chemistry: (4th Ed) Wiley-Blackwell
6. Cleydon, J. , Greeves, N. , Warren, S. and Wolthers, P. 2001 Organic Chemistry: Oxford (2001)
7. Paquette L. A. and Benjamin W. A. 1968 Modern Heterocyclic Chemistry by W.A., Inc.,
8. Finar I. L. 1968 Organic Chemistry Vol II, ELBS.
9. Gilchrist, T. R. 1989 Heterocyclic Chemistry.

CHE-PG-C203: Physical Chemistry 4 credits

Unit I: Statistical Thermodynamics

Concepts of distribution, thermodynamic probability and most probable distribution. Ensemble averaging, postulates of ensemble averaging. Canonical and microcanonical ensembles, Boltzmann distribution of particles.
Partition function: translational, rotational and vibrational partition functions, thermodynamic properties of ideal gases in terms of partition function.

Unit II: Quantum Mechanics

Fundamentals: Review of essential mathematical concepts. Origin of the quantum theory. Postulates of quantum mechanics and Schrödinger equation; its application on some model systems viz., free-particle and particle in a box, tunneling, the harmonic oscillator, the rigid rotator, and the hydrogen atom. The variation theorem; linear variation principle;
Approximation Methods: Stationary perturbation theory for non-degenerate and degenerate systems with examples. Variation method. Ground state of He atom. Time-dependent perturbation theory. Radiative transitions. Einstein coefficients.
Atomic Structure: Many electron wave functions. Pauli Exclusion principle. Helium atom. Atomic term symbols. The self-consistent field method. Slater-type orbitals.
Group Theory Definition of group, symmetry, point groups, representation of group, orthogonality theorem, irreducible representation, character table, direct sum, direct product, derivation of projection operator

Unit III: Rotation and Vibration of Diatomic Molecules

Selection rules. A review of MW and IR spectroscopy. Symmetry properties and nuclear spin effects. Raman effect: Rotational and vibration-rotational transitions. Polarization of Raman lines. Vibration of polyatomic molecules– normal coordinates.

Electronic Spectroscopy: Absorption and Emission of radiation. Selection rules. Line shapes and widths. Electronic spectroscopy of diatomic molecules. Franck-Condon factor. Dissociation and pre-dissociation. Rotational fine structure. Lasers and Laser spectroscopy.

Unit IV: Reaction Dynamics

Methods of determining rate laws, collision theory of reaction rates, Arrhenius equation and activated complex theory. Potential energy surfaces. Unimolecular reactions and their treatments (Lindemann-Hinshelwood and Rice-Ramsperger-Kassel-Marcus [RRK], RRKM theory) Experimental Methods: Enzyme kinetics, studies of fast reactions by flow method, relaxation method, flash photolysis and NMR. Techniques: Flow techniques.
General consideration of gas and solution phase fast reactions: Gas phase and solution phase reactions, Reactions at microsecond and nanosecond scale, ultrafast reactions: reactions at picoseconds and femtoseconds scale.

References

1. Atkins, P. W. 2002 Physical Chemistry, 7th Edition, Oxford University Press, New York.
2. Maczek, A. Statistical Thermodynamics, Oxford University Press Inc., New
3. Reif, F, 1985 Fundamental of Statistical and Thermal Physics McGraw Hill, International edition.
4. Barrow, G. M. Introduction to Molecular Spectroscopy McGraw Hill
5. Pilar, F. L. 1990 Elementary Quantum Chemistry 2nd Edition, McGraw - Hill Publishing Company.

6. Atkins P. W. and Friedman, R. S, 1997, Molecular Quantum Mechanics 3rd Edition, Oxford Univ. Press.
7. Laidler, K. 1995 Chemical Kinetics Harper and Row.
8. Levine, I. N. 2002 Physical Chemistry, 5th Edition, Tata McGraw Hill Pub. Co. Ltd., New Delhi.
9. Brouard, M. 1998 Reaction Dynamics, Oxford University Press, Oxford.
10. Levine R.D. and Bernstein, R.B. 1987 Molecular Reaction Dynamics and Chemical Reactivity, Oxford University Press, Oxford.

CHE-PG-C204: Practical II 4 credits

Organic Chemistry Experiments

A. Extraction of Organic Compounds from Natural Source (Any three)

A.1. Isolation of caffeine, an alkaloid, from tea leaves.

A.2. Isolation of casein from milk (the students are required to try some typical colour reactions of proteins)

A.3. Isolation of lactose from milk (purity of sugar should be checked by TLC and PC and Rf value reported.)

A.4. Isolation of nicotine dipicrate from tobacco.

A.5. Isolation of cinchonine from cinchona bark.

A.6. Isolation of piperine from black pepper.

A.7. Isolation of lycopene from tomatoes.

A.8. Isolation of -carotene from carrots.

A.9. Isolation of oleic acid from olive oil (involving the preparation of complex with urea and separation of linoleic acid.

A.10. Isolation of eugenol from cloves.

A.11. Isolation of limonine from citrus rinds.

A.12. Extraction and identification of DNA from green peas and onions

B. Spectro-photometric (UV/VIS) Estimations (Any Three)

B.1. Amino acids

B.2. Proteins

B.3. Carbohydrates

B.4. Cholesterol

B.5. Ascorbic acid

B.6. Aspirin

B.7. Caffeine

C. Synthesis of organic compounds, purification and characterization by chemical analysis, IR, UV-Vis, PL, NMR spectral analysis and mass spectral analysis: (Any three)

C.1. Synthesis of fluorescein, a classic fluorescent dye
C.2. Synthesis and chemiluminescence of luminol
C.3. Diels-Alder reaction of anthracene and maleic anhydride
C.4. Aspirin synthesis: Conventional and with microwave assistance
C.5. Sand Meyer's reaction: p-Chlorotoluene from p-chlorotoluidine.
C.6. Cannizzaro reaction using 4-chlorobenzaldehyde
C.7. Preparation of 1,3,5 tribromobenzene from analine
C.8. Acetoacetic ester condensation

Books Recommended:

C.8.1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.

C.8.2. Addison Ault Techniques and Experiments for Organic Chemistry 6th Ed. University Science Books (1998).

C.8.3. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry 4th Ed. Orient Longmans (1990).

C.8.4. Vogel, A. I. Vogel's Textbook of Practical Organic Chemistry 5th Ed. (revised by
A.R. Tatchell et al.) Wiley (1989) ISBN 0582-46236-3

Semester III

CHE-PG-O301: Instrumental Techniques 4 credits

Unit I: Chemical Instrumentation

Elementary Electronics, Simple integrated circuit, Semiconductor, Power supply, transformer, operational amplifier, Lock-in amplifiers, Detectors (Oscilloscope and recorders), transducers, Rectifiers, Signal to noise ratio, Electronic components (Resistors, capacitors, inductors, transistors), Measuring instruments for pressure, temperature, pH, speed, flow, current and voltage. Fourier transformation.

Errors in Chemical Analysis and Statistical Evaluation of Data: Systematic and random errors, accuracy and precision, the correlation coefficient, Mean, Median and Modes, variance, standard deviation and significant figures.

Separation Methods: Principle of chromatography, Classifications of chromatography, Techniques of planar and column chromatography, Gas chromatography, High-performance liquid chromatography.

Unit II: UV-Visible Spectroscopy

Principles and Applications: dienes, polyenes, carbonyl compounds and α, β-unsaturated carbonyl compounds. Woodward Hoffman rule and its application in aromatic compounds. Infrared Spectroscopy: Vibration modes. Absorption frequency of common functional groups, electronic and steric effects, effects of Hydrogen bonding. Interpretation of IR spectra.

Raman Spectroscopy: Principles of Raman Spectroscopy and its comparison with IR spectroscopy. Applications of vibrational spectroscopy: Symmetry and shapes of AB_2, AB_3, AB_4, modes of bonding in ambidentate ligands.

Emission Spectroscopy: Principle and application of Fluorescence, phosphorescence, chemi-luminescence

Mössbauer Spectroscopy: Basic principle, conditions for Mössbauer spectroscopy, Spectral parameters (Isomer shift, electric quadrupole interactions, magnetic interactions), temperature- dependent effects, structural deductions for iron and tin complexes, miscellaneous applications.

Unit III: NMR Spectroscopy

Principle, instrumentation and different techniques (continuous wave and Fourier transformed) of NMR spectroscopy, factors influencing chemical shifts of the spectra, anisotropy, spin-spin interactions, coupling constant (J), spin-decoupling, Nuclear Overhauser Effect (NOE),

classification of AB, ABC, AMX and A_2B_2 type couplings, First order spectra, lanthanides shift reagent, spin-spin and spin lattice relaxation processes. Applications. Introduction to ^{13}C NMR,

principles of decoupling, Application of DEPT. ^{1}H- ^{1}H COSY, HETCOR, NOESY, ROESY.

Basic introduction to ^{19}F and ^{31}P NMR and heteronuclear coupling. Solid-state NMR: Basic principles and applications. MRI basics. MRI Contrast agents.

Electron Spin Resonance Spectroscopy: Basic principle, Hyperfine splittings (isotropic systems); the g-value and the factors affecting thereof; interactions affecting electron energies in paramagnetic complexes (Zero-field splitting and Kramer's degeneracy); Anisotropic effects (the g-value and the hyperfine couplings); The EPR of triplet states; Structural applications to transition metal complexes.

Unit IV: Other Spectroscopic Techniques

UV photoelectron spectroscopy, X-ray photoelectron spectroscopy, ESCA and Auger, EDX. Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), Scanning tunnelling microscopy (STM) and Atomic force microscopy (AFM). Cyclic Voltammetry, Inductively coupled plasma emission spectroscopy (ICPE), TGA, DSC, DTA and thermometric titration.

Mass Spectrometry: Introduction, ion production, fragmentation, factors influencing ion abundance, single and multiple bond cleavage, rearrangements, cleavage associated with common functional groups, molecular ion peak, metastable ion peak, Nitrogen rule and interpretation of mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak; Ionization techniques (EI and FAB).

Optical Rotatory Dispersion and Circular Dichroism. Linearly and circularly polarized lights; optical rotatory power and circular birefringence, elipticity and circular dichroism; ORD and Cotton effect, Faraday and Kerr effects

References

1. Strobel, H.A. 1973 Chemical Instrumentation - A Systematic Approach, 2nd Edition, Addison Wesley, Mass.
2. Skoog D.A., Holler F.J. and Nieman, T.A. , 1998 Principles of Instrumental Analysis, 5th Edition, Harcourt Brace & Company, Florida.
3. Hollas, J. M. 2004 Modern Spectroscopy, 4th edition, John Wiley & Sons, Ltd., Chichester.
4. Harris, R. K. 1986 Nuclear magnetic resonance spectroscopy John Wiley and Sons Inc.,New York, NY .
5. R.J. Abraham and J. Fishe and P. Loftus, 1994, Introduction to NMR Spectroscopy John Wiley & Sons.
6. Ladd M. F. C. and Palmer, R. A. 1985 Structure Determination by X-Ray Crystallography Plenum, NY, 2nd Ed.
7. Williams, D B. Carter, C. B. 2008 Transmission Electron Microscopy: A Textbook for Materials Science Springer.
8. Sarid, D. 1991 Scanning Force Microscopy With Applications to Electric, Magnetic and Atomic Forces New York, Oxford University Press
9. Chary, K. V. R. and Govil, G. 2008 NMR in biological systems: from molecules to human, Springer
10. Pecsok, R. P., Shields, L. D. , Cairns T. and William, L.C. Mc, 1976, 2nd Edition, John Wiley, New York.

CHE-PG-C304: Practical III 4 credits

Physical Chemistry Experiments

A. Electrochemistry and Kinetics: (Any three)

1. Analysis of halide mixture by differential potentiometry
2. Degree of hydrolysis of urea hydrochloride by kinetics method.
3. Equilibrium constant of $KI + I_2 \leftrightarrow KI_3$ by distribution method.
4. Kinetics of the iodide-hydrogen peroxide clock reaction
5. An experiment to determine the energy of activation, Ea
6. Determination of the amount of calcium in milk powder by EDTA complexometry
7. Estimation of iodine in iodized common salt using iodometry
8. Determination of phosphoric acid in soft drinks
9. Antioxidant property of Tea (DPPH method).

B. Physical and Analytical methods: (Any seven)

Experiments based on

1 UV - Visible spectroscopy with application
2 Fluorescence Spectroscopy with application
3 Infrared Spectroscopy
4 EPR Spectroscopy

5 NMR Spectroscopy
6 Solvents effects in spectra
7 Differential Scanning Calorimetry
8 High Pressure Liquid Chromatography
9 Spectroscopy Instrumentation
10 Cyclic voltametry
11 Enzymetic reaction
12 Semiconductor materials (Quantum dots)
13 Metal Nanoparticles
14 Polymer
15 Magnetic nanoparticles
16 Ionic liquids
17 Liquid crystals
18 Optical materials
19 Carbon based nanomaterials
20 Paper and column chromatography of plant pigments
21 Acetylation of ferrocene and its purification by column chromatography
22 Ternary phase diagram
23 Determination of surface tension by differential capillary method.
24 Determination of molecular weight of a macromolecule by viscometry.
25 Determination of molecular weight by Victor Meyer's method.
26 Cryoscopy and determination of degree of dissociation.
27 Determination of g-value by ESR method.
28 Analysis of a UV spectrum, Raman spectrum, IR spectrum, NMR spectrum and EPR spectrum. Calculation of oscillator strength and transition moment.
29 Potentiometric titrations using the pH meter and determination of pI
30 Conductometric titrations and determination of dissociation constant
31 Determination of Phosphoric acid in soft drinks

Books Recommended:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. Daniels, F., Williams, J. W., Bender, P., Alberty, R. A., Cornwell, C. D. & Harriman, J. E. Experimental Physical Chemistry, McGraw-Hill (1962).
3. Das & R. C. & Behera, B., Experimental Physical Chemistry, Tata McGraw-Hill Publishing Co. Pvt. Ltd. (1993).
4. Shoemaker, D. P., Garland, C. W. & Nibler, J. W. Experiments in Physical Chemistry, McGraw-Hill: New York (1996).
5. Day, R. A., Jr. & Underwood, A. L. Quantitative Analysis 3rd Ed. Prentice-Hall India Pvt. Ltd.: New Delhi (1977).
6. Burns, D. T. & Rattenbury, E. M. Introductory Practical Physical Chemistry Pergamon Press (1966)
7. Harris, D. C. Quantitative Chemical Analysis 6th Ed. W. H. Freeman & Co. (2002).

8. Willard, H. H., Merritt, L. L., Dean, J. A. & Settle, F. A. (Eds.) Instrumental Methods of Analysis - 7th Ed., Wadsworth Publishing (February 1988) ISBN 0534081428
9. EDTA Titrations –F.Laschka
10. Experimental Physical Chemistry by A.M. Halpern, 2nd Ed., Prentice Hall, 1997.

Electives

CHE-PG-E301: Chemistry of Inorganic Materials 4 credits
Inorganic Chemistry Elective I

Unit- I: Solid State Chemistry:
Bonding in solids and Crystal energetic. Crystal classifications, Madelung constant and Lattice energy. Electronic properties and Band theory of solids. Free electron model, Refinement to simple band theory- k-space and Brillouin Zones, Band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, Doped semiconductors, p-n junctions.

Unit- III: Structure of Solids
Crystal systems; Designation of crystal faces, lattice structures and unit cell; Bragg's law; X-ray diffraction by crystals; Close packing, radius ratio rules, calculation of some limiting radius ratio values; Structures of NaCl, KCl, ZnS, CsCl and CaF_2; Stoichiometric and nonstoichiometric defects, impurity defects, semi-conductors. Packing in solids, Crystal structures of representative systems, Pervoskites, Silicates and Zeolites, Cements, Glasses, Quasicrystals, Nanostructures.

Unit III: Supramolecular Chemistry
Origin of supramolecular chemistry-"Chemistry beyond the molecules". Concepts and terminology of supramolecular chemistry. Natural types of supramolecular interactions (Hydrogen bonding, van der Waal"s interaction, π-stacking, CH---π interaction. supramolecular chemistry in inorganic perspective. Inorganic crystal engineering and design principle of metal organic framework (MOF). Application of MOFs in material science.

Unit IV: Metallomesogens and Inorganic Polymers
Basic concepts, types of meso-phases, synthetic strategies, characterization and applications. Inorganic Polymers: Classification, Types of Inorganic Polymerization, Comparison with organic polymers, Boron-oxygen and boron-nitrogen polymers, silicones, coordination polymers, sulfur-nitrogen, sulfur-nitrogen-fluorine compounds, chalcogenide clusters – binary and multi- component systems, homolytic inorganic systems.

References

1. Greenwood N. N. and. Earnshaw, A. 1997 Chemistry of the Elements, 2nd Edn., Butterworth Heinemann, London.
2. Lehn J. M., 1995 Supramolecular Chemistry, VCH, Weinheim.
3. Kahn O., 1993 Molecular Magnetism, VCH, Weinheim.

4. Cotton, F. A., Wilkinson, G., Murillo C. A. and Bochmann, M. , 2003, Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons (Asia), Singapore.
5. Mark, J. E., Allcock, H. R. and West, |R. 2004 Inorganic Polymers, 2nd Edn., Oxford University Press.
6. Huheey, J. 1993 Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York
7. Miessler G. L. and Tarr, D. A. 1999 Inorganic Chemistry, 2nd Edn., Prentice Hall International Inc., London.
8. Serrano, J. L. 1996 Metallomesogens, VCH, Weinheim.

CHE-PG-E302: Organometallic Chemistry 4 credits
Inorganic Chemistry Elective II

Unit I: Complexes of σ- donor π-acceptor ligands:
(a) σ–bonded systems: metal-alkyls, -aryls and -hydrides, stability, preparation and reactivity, metal-carbonyls, metal-phosphines, metal-nitrosyls, metal-isocyanides: structures, reactivity and bonding, Metal-carbenes, metal-carbynes, Fischer carbenes, Schrock carbenes, complexes with N-heterocyclic carbenes, olefin metathesis
(b) π-Complexes of Unsaturated Molecules: Structure, bonding and reactivity of alkene, alkyne, allyl, dienyl and trienyl complexes; reactions with special reference to organic synthesis.

Unit II: Metal Carbonyls and Metal Clusters
Metal carbonyls: Synthesis, structure and reactivity; bonding in metal carbonyls, variants of CO bridging, vibrational spectra of metal carbonyls, principal reaction types of metal carbonyls. Low nuclearity (M3-M4) and high nuclearity (M5-M10) carbonyl clusters. Metal-metal bonding(MO), skeletal electron counting. Wade-Mingos Lauher rule, isolobal analogy. Halide clusters of Nb, Ta, Mo, W, Re. Synthesis, structure and bonding. Interstitial Clusters-hydrides, carbides and nitrides.

Unit III: Organometallic reaction mechanism:
Ligand Exhange, Associative mechanism: Brookhart Polymerization Catalysts, 16 electron rule Dissociative meachanism: Oxidative addition;, Reductive elimination; transmetallation: Suzuki-Miyaura, Migratory Insertion / De-insertion, Agostic interaction, β-Hydride Elimination, Wacker Oxidation, Heck Arylation

Unit IV: Homogeneous & Heterogeneous Catalysis
Applications of organometallics in organic synthesis: C-C bond coupling reactions (Heck, Sonogashira, Suzuki), reduction using transition metal hydrides, asymmetric hydrogenation. Alkene isomerization; Hydrogenation; Hydroformylation; Monsanto acetic acid process; Alkene polymerization; Cross coupling reactions; Metathesis; C-H activation and functionalization; Buchwald-Hartwig Reaction and Metathesis reaction, Oxidation of olefins;

References:

1. Huheey, J. 1993 E. Inorganic Chemistry, 4th Edn., Addison Wesley Pub. Co., New York.
2. Cotton F. A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John- Wiley & Sons, New York.
3. Crabtree, R.H. 1988 The Organometallic Chemistry of the Transition Metals, 1st Edn., John-Wiley & Sons, New York.
4. Shriver , D. F. and Atkins, P. W. 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
5. Greenhood, 1976 Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
6. Cleydon, J. , Greeves, N. , Warren, S. and Wolthers, P. , 2001 Organic Chemistry: Oxford
7. Collman, J. P. , Hegedus, L. S. , Norton J. R and Finke, Richard G. 1987 Principles and Applications of Organotransition Metal Chemistry, 1st Edn., University Science Books, Mill Valley, California.
8. Elschenbroich, Ch. and. Salzer, A, 1991 Organometallics: A Cosize Introduction, 2nd Edn.,VCH
9. Mehrotra, R. C. and Singh, A, 2004 Organometallic Chemistry: A Unified Approach, New age international limited, 2nd Edn.

CHE-PG-E311: Advanced topics in Organic Chemistry 4 credits
Organic Chemistry Elective I
Unit: 1

Special topics in stereochemistry:
General consideration of molecular asymmetry and dissymmetry, Determination of Special chiralities- axial, planner and helical chiralities, determination of their absolute configurations.
Topicities and relations, pseudo chirality, prochiral faces of carbonyl and alkenes. Meaning absolute and relative stereo chemistry of a molecule. chemical transformation,
Shape and stability of various conformations of molecules of different ring sizes and containing different functional groups, conformation and reactivity in cyclohexanes and decalin systems. quasiracemates, dynamic stereochemistry , atropisomerism of biphenyls.
Stereoselective synthesis: Different methods to introduce chirality or generate new chiral centres in a molecule. Asymmetric synthesis using chiral substrate, chiral auxiliaries, chiral reagents and chiral catalysts with various examples. Advantages and disadvantages of each of these techniques., Application of each of these techniques in synthesis of various natural products.

Unit II: Synthesis and mechanism of action of some new generation antibiotics.
New generation antibiotics/antibacterial agents: Synthesis and mechanism of action of (i) fluoroquinolones – norfloxacin, ciprofloxacin, O-floxacin, levofloxacin (ii) anti AIDS drugs – AZT, lamivadine (iii) antihypertensive agent – captopril (iv) calcium channel blocker – amlodipine (v) gastric secretion inhibitor – omeprazole and its mechanism of action (vi) drug for impotency – sildenafil and its mechanism of action.,

Unit III: Synthesis and application of organic materials

Organic Materials: Synthesis of Fullerenes, Carbon nanotubes, graphenes and various conducting polymers.
Conducting organics - Conducting polymers. Organic superconductors.
Liquid crystals: mesomorphic behaviour, optical properties of liquid crystals, display devices. Organic light emitting diodes.

Unit IV: Green Chemistry and solid phase reactions

Green Chemistry: Overview. Set of principles of green chemistry, green synthetic methods, catalysis, organics reactions in aqueous media, ionic liquids, supercritical fluids and under microwave radiations. Solvent from organics reactions, solid phase organics reaction and catalysis.

References:

1. Stereochemistry of Organic Compounds,.Eliel E.L. and Wilen, S.H., Wiley Interscience, New York, 1994
2. Stereochemistry of Organic Compounds. Principles and Applications. D. Nasipuri. John Wiley & sons, Chichester, 1991.
3. Classics in Stereoselective Synthesis, Wiley, Erick M. Carreira, Lisbet Kvaerno 2008
4. Stereoselective Synthesis in Organic Chemistry, Atta-ur-Rahman, Zahir Shah; Springer- Verlag New York, 1993
5. Stereoselective Synthesis: A Practical Approach, 2nd, Revised and Updated Edition; Mihály Nógrádi, Wiley; 1994
6. Antibiotics: Targets, Mechanisms and Resistance; Claudio O. Gualerzi, Letizia Brandi, Attilio Fabbretti, Cynthia L. Pon; Wiley-VCH; 2013
7. Antibiotics: Challenges, Mechanisms, Opportunities; Christopher J. Walsh, T. Wencewicz; 2016 ASM Press; 2016
8. Carbon Nanotubes and Related Structures: Synthesis, Characterization, Functionalization, and Applications Dirk M. Guldi, Nazario Martín ; WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim; Academic Press; 2010
9. Flat Panel Displays, Advanced Organic Materials; S.M. Kelly; RSC Materials Monographs; The Royal Society of Chemistry 2000
10. Conducting Polymers, Fundamentals and Applications: A Practical Approach; Prasanna Chandrasekhar; Springer Science & Business, 2013
11. Green Chemistry: An Introductory Text:, Lancaster, M. Royal Society of Chemistry; 2002

CHE-PG-E312: Instrumental Techniques for Organic Chemistry 4 credits
Organic Chemistry Elective II

Unit I Further topics in ^{1}H NMR Spectroscopy and ^{13}C NMR spectroscopy

^{1}H NMR Spectroscopy: Chemical exchange, effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between two, three, four and five nuclei (first order spectra), factors effecting coupling constant "J", classification of spin system like AB, AX, AX2, ABX, AMX, ABC, A2B2. Spin decoupling, Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic 4 double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear overhauser effect (NOE), resonance of other nuclei like ^{31}P, ^{19}F.

^{13}C NMR spectroscopy: FT NMR, Types of ^{13}C NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, Homo nuclear (^{13}C-^{13}C) and Hetero nuclear (^{13}C-^{1}H)coupling constants.

Unit II Mass spectrometry and 2D NMR Techniques:

Mass Spectrometry: Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupoule mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors influencing ion abundance, single and multiple bond cleavage, rearrangements, Nitrogen rule and interpretation of mass spectra, effect of isotopes on the appearance of mass spectrum, recognition of the molecular ion peak;

2D NMR Techniques: General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)- Homo COSY (^{1}H-^{1}H), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

Unit III

Structure elucidation through the application of UV, IR, PMR, CMR, 2D NMR and Mass spectrometry.
(Including reaction sequences)

Unit IV

Molecular dyssemetry and chiroptical properties

Linear and circularly polarized lights, circular birefringence and circular dichroism, ORD and CD curves, Cotton effects, Faraday and Kerr effects. The axial halo-ketone rule, Octent diagrams, Helicity and Lowe's Rule. Application of ORD and CD to structural and stereochemical problems.

Separation techniques:

Fundamental principles, theory, instrumentation and application of Gas-liquid chromatography, HPLC, Size Exclusion chromatography, GC-MS, LC-MS, UPLC, HPTLC, Ion Pair & Ion Exchange Chromatography and Supercritical Fluid Chromatography.

References:

1. Introduction to Spectroscopy – D. L. Pavia, G.M. Lampman, G. S. Kriz, 4th Ed. Cengage Learning, 2008
2. Spectrometric identification of organic compounds R. M. Silverstein, F. X. Webster, David Kiemle, David L. Bryce; 8th Ed. John Wiley and Sons. 2014
3. A Complete Introduction to Modern NMR Spectroscopy, Roger S. Macomber, Wiley, 1997
4. High-Resolution NMR Techniques in Organic Chemistry 3rd Edition Timothy D.W. Claridge Elsevier Science, 2016
5. Modern NMR Spectroscopy: A Guide for Chemists; Second Edition; Jeremy K. M. Sanders, Brian K. Hunter; Wiley, 1993
6. Solving Problems with NMR Spectroscopy, 2nd Edition; Atta-ur-Rahman Muhammad Choudhary Atia-tul- Wahab; Academic Press, 2015
7. Eberhard Breitmaier. Structure elucidation by NMR in organic chemistry. A practical guide. Wiley, Chichester, 2002
8. Guide to Fluorine NMR for Organic Chemists, 2nd Edition, William R. Dolbier, Jr.,Wiley, 2016
9. Organic Structures from Spectra, Fifth Edition, L D Field, S Sternhell, J R Kalman John Wiley and Sons Ltd. 2015
10. Organic Structures from 2D NMR Spectra, L. D. Field, H. L. Li, A. M. Magill
11. Phosphorus-31 NMR Spectroscopy A Concise Introduction for the Synthetic Organic and Organometallic Chemist, Olaf Kühl, Springer
12. Organic Structure Determination Using 2-D NMR Spectroscopy, A Problem-Based Approach Jeff rey H. Simpson, Academic Press, 2008
13. Introduction to Modern Liquid Chromatography, Third Edition; Lloyd R. Snyder, Joshep J. Kirkland, John W. Dolan, A John Wiley & Sons, Inc., Publication, 2010
14. Chiral Chromatography, Thomas E. Beesley, Raymond P.W. Scott, Wiley,
15. Mass Spectrometry, Principles and Applications, Third Edition, Edmond de Hoffmann
16. Mass Spectrometry in Medicinal Chemistry; Klaus T. Wanner, Georg Ho¨fner, Wiley, 2007
17. ManMohan Srivastava, High-Performance Thin Layer Chromatography (HPTLC) Springer Heidelberg Dordrecht London New York, 2011
18. LC/MS Applications in Drug Development, Mike S. Lee, Dominic M. Desiderio, Nico M. Nibbering, Wiley Interscience, 2002
19. Ord and Cd in Chemistry and Biochemistry, 1st Edition, Pierre Crabbe, Academic Press, 1972
20. Basic Gas Chromatography, 2nd Edition, Harold M. McNair, James M. Miller, Wiley, 2009
21. Practical Gas Chromatography, A Comprehensive Reference Dettmer-Wilde, Katja, Engewald, Werner Springer 2014
22. Gas Chromatography and Mass Spectrometry: A Practical Guide, 2nd Edition, O. David Sparkman Zelda Penton Fulton Kitson, Academic Press, 2011

CHE-PG-E321: Nanochemistry 4 credits

Physical/ Inorganic Chemistry Elective I

Unit I

Concept of length scale, de Broglie wavelength in a semiconductor, Exciton Bohr Radius, Quantum confinement, Density of states, The Fermi Energy, Fermi Velocity and Kubo gap, The Drude-Lorentz Model, Electron mean free path in metals. Super paramagnetic limit in magnetic nanoparticles. Wave particle duality in C_{60}. Basic crystallography, unit cell, bravais lattice, Miller indices, planes, crystallographic directions, Single element crystals (SC, FCC, BCC), diamond structure, Zinc blende, Rock salt, Wurtzite, Spinel, Rutile, Perovskite, surface to volume ratio, calculation of density using unit cell approach. Debye Scherrer equation. Concept of concentration, Determination of molar extinction coefficient. Surface defects, Surface oxidation. Chemistry of small surfaces: Curvature and neighboring-charge effects on chemical reactivity and equilibria (pKa's, redox potentials), Effect on melting temperature.

Unit II Nucleation and growth:

Classical Theory, Monodispersity, Lamer Plot, Ostwald ripening, Digestive Ripening Homogeneous vs. heterogeneous nucleation and applications of nanomaterials, Anisotropic growth and shape control, Catalyzed (seeded) growth, Nanocrystal doping, solid solutions and Vegard's rule. Non-classical growth. Effect of precursor reactivity and stability on size. Unusual precursor kinetics in III-V semiconductor nanocrystal formation.

Unit III: Synthesis and characterization

Basics of CVD, sol-gel, microemulsion, template and hydrothermal methods. Hot injection (Bawendi and Murray method), heating up, Ion-exchange, Doping, Influence of Precursor reactivity. Reaction kinetics and influence of reaction parameters on the synthesis of CdSe, InP, PbS, Au, Fe_3O_4, $CH_3NH_3PbCl_3$. Synthesis and functionlaisation of Carbon nanotubes, Fullerenes and Graphenes. Core/shell synthesis, SILAR. Purification techniques. Phase transfer: solid phase, solution phase. Surface functionliastion with small molecules, drugs, antibody, cell penetrating peptide, contrast agents. Role of Linkers.

Optical characterization: Absorption and photoluminescence (PL & PLE) spectroscopes, steady-state vs. fast spectroscopy, dynamic light scattering.

Structural characterization: XRD, TEM, AFM, Deviations between bulk and near-surface crystal structures

Unit IV: Properties and application

Quantum dots: Colloidal quantum dots, Optical properties of II-VI (CdSe, CdTe, ZnS), III-V (InP and InAs) and IV-VI (PbS and PbSe) colloidal quantum dots, Perovskites. Photostability of QDs in solution, thin film. Surface passivation, Core/shell nanocrystals. Determination of band

gap. Application in solar cell, LED and bioimaging. Magnetic nanoaprticles: Single domain. Multiple domain. Superparamagnetism. Finite size effects in magnetic nanoparticles, superparamagnetic limit, Neel-Brown expression, Blocking temperature. Properties of Fe_3O_4, Ni, FePt, nanoparticles. Fe_3O_4 as MRI T2 contrast agent. Application in biology and magnetic recording. Metal nanoparticles: Surface Plasmon resonance in Au nanoparticles. Surface Plasmon resonance, Mie theory of metal nanoparticles, Application in biology. Crystal structure of Co nanoparticles. Carbon based materials: Properties of C60, carbon nanotubes, fluorescence in carbon dots and fullerene. FRET

References

1. Kuno, M. Introductory Nanoscience, 2011, Taylor & Francis Group.

2. Rigach, A. L. (Editor), Semiconductor nanocrystal quantum dots: synthesis, assembly and applications

3. Klimov, V. I. Semiconductor and Metal Nanocrystals: Synthesis and Electronic and Optical Properties (Optical Science and Engineering)

4. Thanh, N.T. K. and Sayed, M. A. 2012 El Magnetic Nanoparticles: From Fabrication to Clinical Applications

5. Huck, W. T. and Huck, Wilhelm T. S. (Editor) Nanoscale Assembly: Chemical Techniques

6. Dresselhaus, M. S, Dresselhaus, G. and Avouris, P. Springer-Verlag. Carbon Nanotubes : Synthesis, Structure, Properties, and Applications

7. Acklin, B. and Lautens, E. Magnetic Nanoparticles: Properties, Synthesis and Applications

8. Taurozzi, J. S 2011 Nanoparticle-polymer composite membranes: Synthesis, characterization, and environmental applications.

9. Karn, B. Colvin, V. and Alivasatos, P. 2004 Nanotechnology and the Environment.

10. Zhou, B. Hermans, S., Somorjai, G. A. (Editors)Nanotechnology in Catalysis Volumes 1 and 2

CHE-PG-E421: Advanced Statistical Thermodynamics 4 credits
Physical Chemistry Elective III

Unit I: Statistical Mechanical ensembles Grand Canonical and other ensembles. Statistics of ideal classical and quantum systems: Ideal Bose system (Photons gas, Phonon gas, Helium Gas), superfluidity, Ideal Fermi system, Ideal Gas (Monoatomic, Diatomic gases), Chemical Equilibria in gases, Electrons in metals

Unit II: Statistical Mechanics of Interacting systems: Classical and Quantum – Calculation of partition function for low densities, Alternative derivation of van der Waals equations, Cluster expansion for classical systems, Equation of state. Cluster expansion for quantum systems Virial expansion of equation of state, Imperfect Bose Gas

Unit III Statistical Thermodynamics of Solids and liquids: Hard sphere fluid, Born Green equation, Integral equation. liquid crystal, Florry-Higgins polymer solution theory, Einstein's theory, Debye theory, Superconductivity in metals, Ginzberg-Landau theory of uperconductivity.

Unit IV: Phase transition and Non-equilibrium statistical thermodynamics

Ising model., Lattice gas, Mean field theory, Kaanoff transformation, Renormalization group theory, Langevin equation, Fluctuation-dissipation theorem, Fokker-planck equation, Onsager's regression hypothesis and time correlation functions, response function.

References:

1.Hill T. L., An Introduction to Statistical Thermodynamics: Dover Publications, New York
2.Chandler D. Introduction To Modern Statistcal Mechanics: Oxford University, Press, New York
3.Reif F., Fundamentals of Statistical and Thermal Physics, Levant Books, Kolkata
4.Sinha S. K., Introduction to Statistical Mechanics, Narosa Publishers

Semester IV

CHE-PG-E401: Magnetochemistry 4 credits
Inorganic Chemistry Elective III

Unit I: Magnetochemistry-I: Magnetic properties of substances, orbital and spin angular momentum of electrons, paramagnetic moment and magnetic susceptibility. Paramagnetic and diamagnetic materials, ferromagnetism, ferrimagnetism, antiferromagnetism, magnetic permeability, magnetic susceptibility, magnetization, classical theory of diamagnetism and paramagnetism, diamagnetism and Pascal"s constants, zero-field splitting, spin-orbit coupling. Determination of magnetic susceptibility by these methods: Gouy, Faraday, NMR method and SQUID.

Unit II: Magnetochemistry-II: Magnetic properties and temperature – The curie and Curie- Weiss law, derivation of Curie law. Microstates, hole formalism, multiplet, multiplet width, Lande interval rule, magnetic moments for different multiplet widths, crystal field diagram, quenching of orbital contribution, high spin/low spin equilibrium. Antiferromagnetic interactions in inorganic compounds: Mechanism like – direct interaction, superexchange interactions and

elucidation with poly nuclear metal complexes as well as oxide and halide salts of transition metals.

Unit III: Magnetochemistry-III: Ferromagnetism and Magnetic domains, Hysteresis, Molecular field theory, magnetic sublattice, Ferrimagnetism, Canting and Weak ferromagnetism Heisenberg and Ising model, Correlation of magnetic and structural properties.

Unit-IV: Magnetochemistry-IV
Magnetic materials, long range ordering, superparamagnetism, molecular magnets, metamagnetism, single chain magnet, magnetic ordering, magnetic behaviour of lanthanides and actinides, design of molecular magnets, physical investigations and applications.
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References

1. Cotton, F.A. and Wilkinson, G. 1999 Advanced Inorganic Chemistry, 6th Edn., John Wiley & Sons, New York.
2. Huheey, J. E., 1993 Inorganic Chemistry, 4th Ed., Addison-Wesley Pub. Co., New York.
3. Drago, R. S., 1971 Physical Methods in Inorganic Chemistry, International Edn., Affiliated East-West Press, New Delhi.
4. Shriver, D. F. and Atkins, P. W., 1999 Inorganic Chemistry, 3rd Edn., ELBS, London.
5. Cotton, F. A., Wilkinson, G. and Gaus, P.L., Basic Inorganic Chemistry, 3rd Edition, John Wiley & Sons, New York.
6. Greenhood, 1976, Spectroscopic properties of inorganic and organometallic compounds, Royal Society of Chemistry.
7. Lee, J. D. 1999 Concise Inorganic Chemistry, Blackwell Science.
8. Purcell K. F. and Kotz J. C., 1987 Inorganic Chemistry, W. B. Sauders Com. , Hong Kong.
9. Cotton, F.A. 1990 Chemical Application of Group Theory, 3rd Ed, Wiley-Blackwell.

CHE-PG-E402: Bio-Inorganic chemistry 4 credits
Inorganic Chemistry Elective III

Unit I: Role of alkali and alkaline earth metal ions in biological systems
A. Role of alkali metal ions: Na^+ - K^+ Pump, ionophores and crown ethers. Transport of Na^+-K^+ through membranes
B. Catalysis of phosphate transfer by Mg^{2+} ion,
C. Regulatory role of Ca^{2+} - muscle contraction

Unit II: Heme Proteins
Hemoglobin, myoglobin, hemerythrin, hemocyanin Oxygen activation: Cytochrome P450, Cytochrome c oxidase.
Non-heme proteins: Copper Proteins: Type I, II and III. Copper in cytochrome c oxidase and in respiratory chain, blue copper proteins

Unit III: Proteins with reference to their oxygenation and oxidase activity

Anti-oxidative functions, Nitrate and nitrite reduction (NO_3^- and NO_2^- reductase), Synthetic models of iron-sulfur proteins, molybdo-enzymes – molybdenum cofactors (molybdenum-pterin complexes, nitrogen fixation through metal complexation, nitrogenase, Photosynthesis (PS-I and PS-II).

Unit IV: Metalloenzymes

Zinc enzymes- carboxypeptidase and carbonic anhydrase. Iron enzyme - catalases, peroxidase and cytochrome P-450. Copper enzyme-superoxide dismutase. Molybdenum oxo-transferase enzyme-xanthine oxidase. Urease and hydrogenase, and cyanocobalamine.

Metal ion storage and transport: Ferritin, transferritin, siderophores and metallothionein and hemosiderin.

Chemotherapeutic applications of metal complexes: Pt(II), Pt(IV) complexes and Ru(II), Ru(III) complexes as anticancer drugs, Au complexes as antiarthritis drugs

References

1. Hughes M. N., 1981 Inorganic Chemistry of Biological Processes, 2nd Ed., John-Wiley & Sons, New York.
2. Kaim W. and Schwederski B., 1995 Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, An Introduction and Guide, Wiley, New York.
3. Lippard S. J. and Berg J. M., Principles of Bioinorganic Chemistry, University Science Books.
4. Bertini, I. , Grey H. B., Lippard S. J. and Valentine, J. S. , 1998 Bioinorganic Chemistry, Viva Books Pvt. Ltd., New Delhi.

CHE-PG-E411: Advances in Organic Synthesis 4 credits

Organic Chemistry Elective III

Unit I

Various synthetic approaches to drug discovery:

Combinatorial synthesis, Diversity oriented synthesis, Total synthesis, their importance, utilities, advantages and disadvantages.

Retrosynthetic analysis: Synthesis backwards, disconnections, synthons, choosing disconnections, functional group interconversion, two group disconnections, C–C disconnections, donor-acceptor synthons, natural reactivity and umpolung.

Synthesis: Illustrative synthesis of complex natural products with relevant examples.

Unit II

Important reaction and synthetic tools in organic synthesis:

Multi-component reactions: Ugi, Passerini, Biginelli and Mannich reactions;

Click chemistry: criterion for click reaction, Sharpless azides cycloadditions;

Coupling reactions: Suzuki, Heck, Sonogashira, Stille, Fukuyama, Kumada, Hiyama, Negishi, Buchwald-Hartwig, Noyori, Reppe, Oxo process

Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, applications
Ring formation reactions: Pausan-Khand, Bergman and Nazerov cyclization, Various intramolecular cycloaddition reactions (INC)

Unit III Other important reactions:

Important named reactions: Wittig, Horner-Wordworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions, Titanium-carbene mediated olefination: Tebbe, Petasis and Nysted reagent, Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction.

Current trends in organic synthesis: Organocatalysis, Photoredox catalysis. C-H activation.

Unit IV Photochemistry:
Quantum yields, intersystem crossing, photosensitization and energy transfer reactions. Photochemistry of olefins and carbonyl compounds, photo oxygenation and photo fragmentation, Photochemistry of aromatic compounds: isomerisation, additions and substitutions. Singlet molecular oxygen reactions. Patterno-Buchi reaction, Di-pimethane rearrangement, Hofmann- Loffler-Freytag reaction, Bartons reaction and Photo-Fries rearrangement.,

References:

1. Combinatorial Chemistry: From Theory to Application, Volume 26, Second Revised Edition; Willi Bannwarth, Berthold Hinzen; Wiley-VCH Verlag GmbH & Co. KGaA, 2006
2. Combinatorial Chemistry: Synthesis Analysis, Screening; Günther Jung; WILEY-VCH Verlag GmbH, 1999
3. Diversity-Oriented Synthesis: Basics and Applications in Organic Synthesis, Drug Discovery, and Chemical Biology Andrea Trabocchi, Wiley, 2013
4. Diversity-oriented Synthesis of Alkaloids for Chemical Genetic Screening; Alexander Merton Taylor Harvard University, 2007
5. Organic chemistry; Clayden, J., Greeves, N. , Warren, S. and Wothers, P.; Oxford University Press, 2000
6. Multicomponent Reactions in Organic Synthesis; Jieping Zhu, Qian Wang, Mei-Xiang Wang; Wiley-VCH Verlag GmbH & Co. KGaA, 2015
7. Multicomponent Reactions: Concepts and Applications for Design and Synthesis; Raquel P. Herrera, Eugenia Marques-López; Wiley, 2015
8. Advance Organic Chemistry; 5th Ed. Carey F. A. and Sundburg R. J.; Springer, 2007
9. Strategic Applications of Named Reactions in Organic Synthesis; Laszlo Kurti Barbara Czako; Academic Press; 2005
10. Name Reactions and Reagents in Organic Synthesis, Second Edition; Bradford P. Mundy, Michael G. Ellerd, Frank G. Favaloro, Jr; John Wiley & Sons, Inc., 2013
11. C-H Bond Activation in Organic Synthesis; Jie Jack Li; CRC Press 2015

12. C-H Activation; Jin-Quan Yu, Zhangjie Shi; Springer; 2010
13. Photoredox Catalysis in Organic Chemistry, Megan H. Shaw, Jack Twilton, and David W. C. MacMillan J. Org. Chem., 2016, 81 (16), pp 6898–6926
14. Organic Photoredox Catalysis; Nathan A. Romero, David A. Nicewicz; Chem. Rev., 2016, 116 (17), pp 10075–10166

CHE-PG-E412: Natural Products and Bio-Organic chemistry 4 credits
Organic Chemistry Elective IV

Unit I: Natural Products

Isoprene Rule, biogenesis and biosynthesis of representative examples. Retrosynthetic analysis of some typical natural products.
Alkaloids: Structure, synthesis, and stereochemistry of Narcotine and Quinine; synthesis and stereochemistry of Morphine, Lysergic acid and Reserpine.
Terpenoids: Camphor, Longifolene, Abietic acid, and Taxol.
Steroids: Cholesterol, Aldosterone and Cortisone.
Prostaglandins and Thromboxanes: Introduction, nomenclature of prostaglandins and thromboxanes; approaches to prostaglandin synthesis; cyclohexane precurors (Woodward synthesis of PGF2a), bicycloheptane precursors (Corey's synthesis of prostaglandins E and F) Oxygen Hetrocycles: Flavonoids, isoflavonoids and biosynthetic pathways. Antioxidant properties of flavonoids.

Unit II: Organotransition Metal Chemistry: Applications to Organic Synthesis

Electron counting, bonding, organometallic reaction mechanism; Homogeneous hydrogenation; Organometallics as electrophiles; Synthetic applications of transition metal alkene complexes: Wacker oxidation. Synthetic applications of complexes containing metal – carbon σ bonds: Heck and related reactions, carbonylation reactions; Synthetic applications of transition metal carbene complexes: Fischer carbene, Schrock carbene, metathesis processes, Tebbe's reagent, Zieglar – Natta reaction; Synthetic applications of transition metal alkyne complexes: Pauson – Khand reaction, cyclooligomerisation; Applications of transition metal complexes in the synthesis of: cyclic enediynes, estrone by Volhardt, clavicipitic acid by Hegedus.

Unit III: Enzymes and Mechanism of Enzyme Action

Classification, isolation and purification. Methods of Enzyme analysis. Two substrate reactions; Enzyme inhibition. Mechanism of action of chymotrypsin, aldolase, alcohol dehydrogenase, and lysozyme.

Co-enzyme Chemistry: Cofactors as derived from vitamins; coenzymes, prosthetic groups, and apoenzymes. Structure and biological functions of coenzyme A, thiamine Pyrophosphate, Pyridoxal phosphate, NAD^+, $NADP^+$, FMN, FAD, lipoic acid, and vitamin B_{12}

Unit IV: Chemistry of Medicinally Important Molecules

Bacterial and animal cells, antibacterial agents – mechanism with reference to β-lactam antibiotics; General method of synthesis of β-lactam ring: synthesis of penicillin, 6-APA, cephalosporin, 7-ACA; Morin – Jackson rearrangement; Structure-activity relationship of penicillin. New generation antibiotics / antibacterial agents: Synthesis and mechanism of action of (i) fluoroquinolones – norfloxacin, ciprofloxacin, levofloxacin (ii) anti AIDS drugs – AZT, lamivadine (iii) antihypertensive agent – captopril (iv) calcium channel blocker – amlodipine (v) gastric secret

Vitamins: Structure and synthesis of Vitamins A, C, Thiamine (B_1), Riboflavin (B_2), Pyridoxine (B_6), Cobalamin (B_{12}) and Vitamin D, Vitamin E, Biotin (H) and Vitamin K.ion inhibitor – omeprazole (vi) drug for impotency – sildenafil etc.

References

1. Bruice T.C. and Bentkovic, S., 1996, Bioorganic Mechanisms, Vol. I & II, W. A. Benjamin, New York.
2. Voet D., Voet J.G. and Pratt CW, 1999 Fundamentals of Biochemistry, John Wiley & Sons, New York .
3. Dugas H. and Penney C., 1981, Bioorganic Chemistry: A Chemical Approach to Enzyme Action, Springer- Verlag, New York.
4. Apsimon J.W., Total Synthesis of Natural Products, Vol. 1-6, Wiley-Interscience Publications, New York.
5. Clayden J. , Greeves N., Warren S., and Wothers P., 2001 Organic Chemistry, Chapter 30, Oxford University Press, Oxford.
6. Burger's Medicinal Chemistry and Drug Discovery, 2003 6th Edn. Donald J. Abraham (Editor), Wiley Interscience
7. Smith M. B., March J., 2000 March's Advanced Organic Chemistry. Reactions, Mechanisms, and Structure 5th Edn, Wiley-Interscience
8. Finar I.L., 1975 Organic Chemistry, Vol. II, 5th Edition Reprinted in 1996, ELBS and Longman Ltd., New Delhi.
9. Lehninger A.L., 1992 Principles of Biochemistry, CBS Publishers, Delhi
10. Mahler H.R. and Cordes E.H., 1971 Biological Chemistry, 2nd Edition, Harper and Row Pub., New York.

CHE-PG-E321: Solid-State Chemistry 4 credits
Physical Chemistry Elective I

Unit I: Solid state Chemistry
Basic Principles and applications
Solid State Reactions: General Principles, Experimental procedure, Co-precipitation a a precursor to solid-state reactions, Kinetics of solid-state reactions, Crystallization of solutions, melts, glasses and gels. Preparation of thin films (chemical, electrochemical and physical

methods), Hydrothermal methods, Growth of single crystals: Czochralski method, Bridgman and Stockbarger methods. Zone Melting. Reactions at solid surfaces.

Unit II: Phase transitions, electronic and magnetic properties

Phase Transitions: Thermodynamic and Burger's classification of phase transition, Kinetics of phase transition- nucleation and growth, T-T-T diagrams, Factors that influence kinetics of phase transition, Martensitic and order-disorder transitions.

Electronic Properties and Band Theory: Electronic structure of solids- band theory, Refinement to simple band theory- k-space and Brillouin Zones, Band structure of metals, insulators and semiconductors, Intrinsic and extrinsic semiconductors, Doped semiconductors, p- n junctions. Concepts of thin film devices. Field effect transistors, photovoltaics, Light emitting diodes.

Magnetic Properties: Classification of materials. Magnetism: Types, determination of magnetic susceptibility. Quantum theory of diamagnetism and paramagnetism. Cooperative phenomena. Magnetic domains. Hysteresis. Concepts of GMR, Solid State storage.

Unit III: Structural characterisation techniques

X- ray Diffraction: Diffraction of X-rays by crystals: The Laue equations and Bragg's law, Definitions related to crystal structure. X-ray diffraction experiments: The powder method and the single crystal method. Reciprocal lattice. Structure factor. Structure factor and intensity. Electron density maps.

Electron diffraction: Scattering intensity versus scattering angle, Wierl equation, measurement technique, elucidation of structure of simple gas phase molecules. Low energy electron diffraction and structure of surfaces.

Neutron diffraction: Scattering of neutrons by solids and liquids, magnetic scattering, measurement techniques. Elucidation of structure of magnetically ordered unit cells.

Solid State NMR: Differences between solid and liquid state NMR, comparison with XRD, Magic Angle spinning, Chemical shielding, J-coupling, Dipolar coupling, Quadrupolar coupling.

Unit IV: High-Tc Oxide Superconductors

Structural features of cuprate superconductors. 1-2-3 and 2-1-4 cuprates; structure. Normal state properties: anisotropy and temperature dependence of electrical resistance.

Superconductingstate: heat capacity, coherence length, relation between Tc and hole concentration in cuprates; mechanism of superconductivity in cuprates. Applications of high Tc- cuprates.

Non-linear materials: Second and third order non-linear effects; molecular rectifiers and frequency doublers; unimolecular electronic devices. Photochromic materials; optical data storage, memory and switches.

References:

1. West A.R. 2003 Solid State Chemistry and its Applications, John Wiley and Sons, Singapore.
2. Azaroff L. V. 1977, Introduction to Solids, Tata McGraw-Hill, New Delhi
3. Massa, W. 2004 Crystal Structure Determination 2nd Ed. Springer.
4. Warren, B. E., 1990 X-Ray Diffraction 1st Ed. Dover Publications (1990).
5. Sands, D. E. 1994 Introduction to Crystallography, Reprint Dover Publications.
6. Tinkham Michael, 2004 Introduction to Superconductivity 2nd Edn, Courier Dover Publications.
7. Rammakrishnan, T.V. and Rao C.N.R. 1999 Superconductivity Today Orient Blackswan.
8. Ashcroft N. W. and Mermin N. D., 1976 Solid State Physics, Brooks Cole; 1st edition
9. Keer H. V. 1993 Principles of the Solid State, New Age International.
10. Chakrabarty D.K., 2010 Solid State Chemistry, New Age Science ltd; 2nd Revised edition.

CHE-PG-E422: Advanced Quantum Chemistry 4 credits
Physical Chemistry Elective I

Unit I: Advanced Quantum Chemistry

Ab initio and Semi-empirical Methods for Closed Shell Systems:
Orbitals, Slater Determinants, The Hartree-Fock Self-Consistent Field Method: The generation of Optimized orbitals, Koopman's Theorem (The Physical Significance of Orbital Energies), The electron correlation energy, Density matrix analysis of the Hartree-Fock Approximation, Natural orbitals, The matrix solution of the Hartree- Fock Equations (Roothaan's equations). Density functional theory, Time-Dependent Density functional theory.
Semiempirical Molecular Orbital Methods I - PI Electron Systems: The Hückel Approximation for Conjugated Hydrocarbons, The Pariser-Parr-Pople Method.Semiempirical Molecular Orbital Methods II - All valence - Electron systems: The Extended Hückel Method, The CNDO Method.

Unit II: Electronic Structure of Linear and non linear Molecule

The Born-Oppenheimer Approximation, The MO - LCAO Approximation, The Hydrogen Molecule Ion, H_2^+, The Hydrogen molecule, Molecular Configuration - Interactions, The Valence Bond Method, The stability of chemical bond, Hellmann-Feynman theorem, Molecular

Perturbation Calculations. Electronic Structure of AH_n molecule: Methane, Ammonia and Water, Hybrid Orbitals: The Ethylene and Benzene Molecules.
The Virial Theorem and Chemical Bonding, The Hellmann-Feynman Theorem, The Electrostatic Theorem.

Unit III: Atom-Radiation Interaction

Electromagnetic field and its interaction with one-electron atoms, Spontaneous emission, Electric dipole approximation, rotating-wave approximation (RWA), density matrix approach, Line intensities, widths and shapes, Rabi Oscillations, atomic coherence, Optical Bloch Equations, Photoionization, Scattering: Partial wave analysis, Phase shifts, The Born Approximation.

Unit IV: Quantum Computation & Information

Computer science, Quantum bits, The EPR Paradox, Bell's Theorem, Quantum algorithms, Quantum information theory, Quantum computers: Physical realization, Entropy and information.

References

1. Levine, I.N. 2000 Quantum Chemistry, 5th edition, Pearson Educ., Inc. New Delhi.
2. Karplus M. and Porter, R. N., 1970 Atoms and Molecules, Benjamin, London.
3. Atkins P.W. and Friedman, R.S., 1997 Molecular Quantum Mechanics, 3rd edition, Oxford University Press. Oxford.
4. Pilar, Frank L. 1990 Elementary Quantum Chemistry 2nd Edition, McGraw - Hill Publishing Company.
5. Mc Quarrie D.A. and Simon, J.D. , 1998, Physical Chemistry: A Molecular Approach, Viva Books, New Delhi.
6. Murrell, J.N. ,. Kettle S.F.A and Tedder, J. M. , 1965, Valence Theory,2nd edition, John Viley, New York.
7. Chandra, A.K. , 1994 Introductory Quantum Chemistry, 4th edition, Tata McGraw Hill, New Delhi.
8. Pualing L. and Wilson, E. B. , 1935 Introduction to Quantum Mechanics with Applications to Chemistry, McGraw Hill, New York.
9. B. H. Bransden and C. J. Joachain, 2003, Physics of atoms and molecules, 2nd edition, Pearson.
10. R. Loudon, 2000, The Quantum Theory of Light, 3rd edition, Oxford University Press.
11. Nielsen and Chuang, 2000, Quantum Computation and Quantum Information, Cambridge University Press.

CHE-PG-E403 Elective Inorganic Chemistry Practical 4 credits

1. Synthesis and characterization of the following (any five synthesis)
a. Pervoskite (bulk and nanoparticles)
b. Prussian blue
c. HKUST-1, $Cu_3(BTC)_2$ metal organic framework
d. Metallic nanoparticles (Ni, Co and Cu)
e. Polyoxometallate (V, Mo and W)
f. Layered materials (In_2O_3 and Fe_2O_3)

Characterization techniques to be used for each experiments (wherever applicable) are XRD, UV-vis, FT-IR, TGA/DTA, Surface Area analysis (BET), Magnetic susceptibility measurements, Cyclic Voltammetry, ICP-MS and AAS.

2. Analysis of known compounds (any two)

a. Cyclic voltammetry, ^{1}H and ^{13}C NMR of Ferrocene

b. ^{13}C-NMR and FT-IR of iron carbonyls

c. TGA measurement of $CuSO_4 . 5H_2O$

d. Surface ligand analysis by TGA and FTIR of nanoparticles

e. Magnetic susceptibility measurements of $Fe(acac)_3$ (Evans method)

f. Assignement of absolute configuration using circular dichroism(CD).

3. Chemistry Communication Skills:

a. How to draw chemical structures- Use of CHEMDRAW. How to write and draw equations (both chemical and mathematical).

b. How to find compound related data in the literature?

c. Use and management of mined data- End note.

d. Use of spectral databases and how to report compound data and procedures. Use of other specialized databases- CCDC, PDB, other nuclei NMR databases.

e. Data integrity and recording experiments in the lab notebook.

f. How to write new and views (reviews)? How to make presentation slides and present reviews to an audience?

References:

f.1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.

f.2. A text book of Quantitative Inorganic Analysis – A. I. Vogel

f.3. A Text Book of Quantitative Inorganic Analysis- A. I. Vogel

f.4. Experimental Inorganic Chemistry - W. G. Palmer

f.5. Synthesis and Characterization of Inorganic Compounds, W.L. Jolly, Prentice Hall.

f.6. Chemistry experiments for Instrumental Methods by Donald T. Sawyer, William R. Heineman & Jalice M. Beebe , John Wiley & Sons ,1984.

f.7. Experimental Physical Chemistry by G. Peter Matthews, Clarendon Press, 1985.

f.8. Handbook of Inorganic Synthesis: G. Brauer

f.9. Inorganic Synthesis: R. B. King

f.10. Synthesis and Technique in Inorganic Chemistry: A Laboratory Manual, Gregory S. Girolami, Thomas B. Rauchfuss and Robert J. Angelici. University Science Books.

CHE-PG-E413 Elective Organic Chemistry Practical 4 credits

Organic Chemistry Experiments

B. Organic Special Practical: Part I

Preparation of organic compounds by typical organic reactions, purification and characterization of the product [by re-crystallization, TLC, PLC, determination of Rf value as required, m.p/b.p.]. Characterization of organic compounds by spectroscopic means.

B. Organic Special Practical: Part II

Multistep Organic Preparation. Extraction and Purification of Natural Products and Biomolecules.

Books Recommended:

1. Elias, A. J., Collection of Interesting General Chemistry Experiments, Orient Longman.
2. Addison Ault Techniques and Experiments for Organic Chemistry 6th Ed. University Science Books (1998).
3. Mann, F. G. & Saunders, B. C. Practical Organic Chemistry 4th Ed. Orient Longmans (1990).
4. Vogel, A. I. Vogel's Textbook of Practical Organic Chemistry 5th Ed. (revised by A.R. Tatchell et al.) Wiley (1989) ISBN 0582-46236-3

CHE-PG-E423 Elective Physical Chemistry Practical 4 credits

Experimental Solid state and Nanomaterials

1. Synthesis and Characterisation of Nanoparticles (Metal, Spinel, Rutile, Zinc blende, Wurtzite Pervoskite)
2. Determination of Molar extinction coefficient of Nanoparticles.
3. Isolation and physical characterization of Fullerene C_{60} from natural sources.
4. Determination of size of nanoparticles using UV-Vis spectrophotometer and X-Ray Diffraction
5. Determination of quantum yield of quantum dots.
6. Solution and solid state ligand exchange in nanoparticles. Computational

Physical

1. Writing and executing computational codes for the following –Radioactive Decay, Other First-Order Reactions etc.
2. Use of quantum mechanical software – Gaussian, MPQC – calculation of energies of molecules.
3. Coding Minimization Algorithms: LBFGS etc.
4. Numerical Methods Roots of Polynomials, Solution of Linear simultaneous equations, matrix multiplication and inversion.
5. Numerical integration.
6. Statistical treatment of data, variance and correlations, Least square curve fitting.

CHE-PG-E404: Project for M.Sc. Thesis 4 credits

Each student has to carry out innovative research on a topic chosen by the student.

Course Objectives:

a) Identification of the problem.
b) Literature review.
c) Exposure to analytical techniques/software
d) Communication skills: Scientific writing, presentation
e) Scientific ethics