

Integrated M.Sc + Ph.D (Dual Degree) Curriculum



Department of Chemistry
Indian Institute of Technology Bombay

DEPARTMENT OF CHEMISTRY

Integrated M.Sc. – Ph.D. programme of the Dept. of Chemistry

First Semester

Code	Name of course	L	T	P	C
CH 423	Organic Chemistry III	2	1	0	6
CH 425	Chemical Bonding and molecular Geometry	2	1	0	6
CH 427	Chemical and Statistical Thermodynamics	2	1	0	6
CH 419	Separation Techniques Lab.	0	0	4	4
CH 433	Physical Chemistry Lab. II	0	0	4	4
CH 438	Chemistry of Main Group Elements	2	1	0	6
CH 481	Computers in Chemistry	1	0	2	4

Contact hours: 23

Credits: 36

Second Semester

Code	Name of course	L	T	P	C
CH 416	Physical Organic Chemistry	2	1	0	6
CH 426	Rate Processes	2	1	0	6
CH 429	Modern Methods of Analysis	2	1	0	6
CH 437	Chemistry of Transition Elements	2	1	0	6
CH 442	Molecular Spectroscopy	2	1	0	6
CH 432	Inorganic Chemistry Lab. III	0	0	4	4
CH 434	Physical Chemistry Lab. III	0	0	4	4

Contact hours: 30

Credits: 42

Summer at the end of 2nd semester

Code	Name of course	C
CH 593	M.Sc. Project	12

Credits: 12

Third Semester

Code	Name of course	L	T	P	C
CH 507	Methods in Organic Synthesis	2	1	0	6
CH 521	Interpretative Molecular Spectroscopy	2	1	0	6
CH 547	Organometallic Chemistry	2	1	0	6
CH 594	M.Sc. Project				18

Contact hours: 09

Credits: 36

Fourth Semester

Code	Name of course	L	T	P	C
CH 402	Thermal and Photochemical Reactions	2	1	0	6
	Elective-I	2	1	0	6
	Elective-II	2	1	0	6
	Elective-III	2	1	0	6
CH 867	Ph.D. : Supervised Learning – 1				10

Contact hours: 12

Credits: 34

Summer at the end of fourth semester

Code	Name of course	C
CH-868	Ph.D.: Supervised Learning - 2	10

Credits: 10

Fifth Semester

Code	Name of course	L	T	P	C
CH 821	Topics in Chemistry	2	1	0	6
CH-831L	Advanced Laboratory Techniques	1	1	4	8
CH0801S	Seminar				4
ES-200/ HS-200		3	0	0	6
HS-699	Communication & Presentation Skill			P	NP

Contact hours: 12

Credits: 24

Departmental electives I to III

Physical Chemistry

CH 504	Computational Chemistry
CH 550	Electrochemistry
CH 552	Interfacial Phenomena
CH 559	Solid State Chemistry and its Applications
CH 560	Quantum Chemistry
CH 576	Statistical Mechanics
CH 584	Biophysical Chemistry
CH 586	Structure and Properties of Materials
CH 5XY	Macromolecular Crystallography

Organic Chemistry

CH-504	Computational Chemistry
CH 510	Heterocyclic chemistry
CH-528	Natural Products
CH-540	Drugs and Biologically active compounds
CH 546	Introduction to Biomolecules
CH-556	Polymer Sciences

Inorganic Chemistry

CH-502	Synthesis and Characterization of Inorganic Compounds.
CH-522	Chemistry of Coordination Compounds
CH-524	Bioinorganic Chemistry
CH-574	Topics in Inorganic Chemistry-I
CH-578	Topics in Inorganic Chemistry-II
CH-582	Inorganic Photochemistry

Investigations of reaction mechanisms. Operational criteria for evaluation of concertedness in potential pericyclic reactions. Photochemical activation and potential energy surfaces. Geometry, dipole moments, acid-base and redox properties of excited states. Uni- and bimolecular deactivations. Quenching mechanisms. Electronic energy transfer mechanisms. Correlation rules and symmetry conservation. Intramolecular (isomerizations, rearrangements and dissociation) and intermolecular (additions) photochemical processes. Electrocyclic reactions- Frontier orbital, orbital and state correlation diagrams, conservation of orbital symmetries, and aromatic transition state approaches to electrocyclic processes. Woodward-Hoffmann rules. Thermal and photochemical electrocyclic processes. Electrocyclic reactions of cations, anions, radicals and radical ions, Metal catalysis. Cycloaddition reactions. FMO, orbital and state correlation diagrams, and aromatic transition state approaches. Various [2+2] [4+2] cycloaddition reactions. Reactivity and regioselectivity in Diels-Alder reactions, Multicomponent cycloadditions. Alder 'Ene Reaction'. Photochemical cycloadditions. Transition metal-catalyzed cycloadditions. Generalized PMO theory for reactivity, regioselectivity and periselectivity in cycloaddition. 1,3-Dipolar cycloadditions. Cheletropic reactions. Sigmatropic reactions- Application of symmetry conservation rules, aromatic transition state and FMO approaches. Various [1,3], [1,5], [1,7], [3,3] and [5,5] shifts. Fluxional Molecules. Sigmatropic rearrangements of charged systems, [3,2] sigmatropic shifts- Ylide rearrangements, Dyotropic reactions. Photo-reactions of nitrobenzyl, azo and diazo compounds, diazirines and azides, caged compounds. Chemiluminescent reactions. Singlet oxygen mediated photoreactions.

Text/References

R. B. Woodward and R. Hoffmann, *The Conservation of Orbital Symmetry*, Academic Press, New York, 1971.

M. J. S. Dewar and R. C. Dougherty, *The PMO Theory of Organic Chemistry*, Plenum Press, New York, 1975.

T. L. Gilchrist and R. C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd edition, Cambridge University Press, Cambridge, 1979.

R. P. Wayne, *Principles and Applications of Photochemistry*, Oxford Science Publications, Oxford University Press, Oxford, 1988.

A. Gilbert and J. Baggot, *Essentials of Molecular Photochemistry*, Blackwell Scientific Publications, Oxford & Boston, 1991.

M. Klessinger and J. Michl, *Excited States and Photochemistry of Organic Molecules*, VCH Publishers, Inc., New York, 1994.

I. Fleming, *Pericyclic Reactions*, Oxford University Press, Oxford, 1998.

A. Rauk, *Orbital Interaction Theory of Organic Chemistry*, 2nd edition, Wiley Interscience, New York, 2001.

S. Sankaraman, *Pericyclic Reactions- A Textbook*, Wiley-VCH, Weinheim, 2005.

H. Maskill (Ed.), *The Investigations of Organic Reactions and Their Mechanisms*, Blackwell Publishing Ltd. Oxford, 2006.

N. J. Turro, J. C. Scaiano and V. Ramamurthy, *Principles of Molecular Photochemistry*, University Science Books, 2008.

CH 416 Physical Organic Chemistry

2 1 0 6

Modern theory of organic structures and bonding. Symmetry-adapted orbitals. Perturbation theory and orbital mixing rules. Buildup approach to large molecular structures. Bonding and structure of reactive intermediates: Carbocations, carbanions, and carbenes. Relation between structure and energetics. Solutions and forces of molecular recognition. Bronsted acid-base chemistry. Lewis acids/bases, electrophiles and nucleophiles. Reactivity, kinetics, and mechanisms. Energy surfaces and transition states. Hammond Postulate. Isotope effects. Hammett plot. Steric and polar effects. Empirical scales of solvent effect. pH and Bronsted relationship. Mechanism and catalysis of proton transfer. General principles of catalysis. Enzyme-catalytic effect and concept of transition-state stabilization. Investigation of organic reaction mechanisms by physical organic approach. Examples illustrating application to investigation of electrophilic/nucleophilic reactions, and enzyme-catalyzed reactions.

Text/References

E. V. Anslyn and D. A. Dougherty, *Modern Organic Chemistry*, University Science, 2005.

A. Pross, *Theory and Physical Principles of Organic Reactivity*, John Wiley, 1995.

A. Rauk, *Orbital Interaction Theory of Organic Chemistry*, John Wiley, 1994.

T. H. Lowry and K. H. Richardson, *Mechanisms and Theory in Organic Chemistry*, Harper and Row, 1976.

CH 418 Organic Chemistry Lab III

0 0 4 4

Chemical separation of ternary organic mixtures and characterization of the components. Simple one or two step preparations involving different techniques. Isolation of natural products.

CH 419 Separation Techniques Lab**0 0 4 4**

Separation by Soxhlet and liquid-liquid extraction. Cation and anion exchange chromatography, column, thin layer and paper chromatography, gas-liquid and gel permeation chromatography. Fractional distillation.

Texts/References

B. L. Karger, L. R. Snyder and C. Horvath, *An Introduction to Separation Science*, John Wiley and Sons, Inc., 1973.

J. A. Dean, *Chemical Separation Methods*, Van Nostrand Reinhold, 1970.

D. J. Pasto and C. R. Johnson, *Organic Structure Determination*, Prentice Hall, 1969.

CH 423 Organic Chemistry-III**2 1 0 6**

A reappraisal of structure, stereochemical principles, properties and reactivity in organic compounds. Study of the following classes of reactions, nucleophilic substitutions, eliminations, electrophilic additions, electrophilic and nucleophilic substitution in aromatic compounds, nucleophilic addition, halogenation, and alkylation of carbonyl compounds. Reactions involving enamines, ester enolates and active methylenes.

Chemistry of conjugated dienes, enones. Pericyclic reactions, FMO theory. Photochemical reactions. Aliphatic and aromatic nitro and amino compounds. Oxidation and reduction reactions.

Texts/References

J. Clayden, S. Warren, N. Greeves, P. Wothers, *Organic Chemistry*, 1st Edition, Oxford University Press, 2000

F. J. Carey and R. J. Sundburg, *Advanced Organic Chemistry, Part A and Part B*, 5th Ed., Springer, 2007

J. March, *Advanced Organic Chemistry*, 3rd edition, McGraw Hill, 1991.

S. H. Pine, *Organic Chemistry*, 5th edition, McGraw Hill, 1987.

CH 425 Chemical Bond and Molecular Geometry

2 1 0 6

Postulates of quantum mechanics; hermitian operators; complete set. Derivation of the uncertainty relations. Exactly solvable problems, orbital angular momentum, and the hydrogen atom. Spin, spin orbitals, and characteristics of a many-electron wave function.

Variation theorem, variation method, the linear variation method, and the non-crossing rule. Applications: Many-electron atoms, self-consistent field, atomic orbitals, Slater Type Orbitals, Slater exponents and the periodic properties of elements; LCAO-MO, Hückel orbitals; Born-Oppenheimer approximation, Potential energy surface, Hellman-Feynman theorem; Hydrogen molecule ion, Hydrogen molecule; Qualitative molecular orbitals for homo- and hetero-nuclear diatomics, isoelectronic principle, hybrid orbitals, and Walsh molecular orbital diagram.

Time-independent perturbation theory - Rayleigh-Schrödinger formulation. Applications: Zeeman effect, Stark effect, crystal field splitting, and simple ligand field treatments.

The valence bond treatment of hydrogen molecule; Resonance; Polarity and dipole moment; Electronegativity; Valence-bond wave functions for polyatomic molecules.

Texts/References

R. McWeeny, *Coulson's Valence*, Oxford University Press, 1979.

D. A. McQuarrie, *Quantum Chemistry*, Oxford University Press, 1983.

I. R. Levine, *Quantum Chemistry*, Prentice Hall India (Ltd), 1995.

S. N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books, 1998.

CH 426 Rate Processes

2 1 0 6

Rates of chemical reactions, rate expressions. Methods of determining rates and orders of reactions. Complex reactions. Collision and transition state theories of chemical reaction rates. Potential energy surfaces and reaction dynamics. Application to unimolecular and bimolecular reactions. Homogeneous catalysis, chain reactions. Photochemical reactions. Fast reactions. Diffusion in solids, liquids and solutions. Chemical oscillations and nonlinear dynamics.

Texts/References

K. A. Connors, *Chemical Kinetics : A Study of Reaction Rates in Solution*, V.C.H. Publications 1990.

J. I. Steinfeld, J. S. Francisco and W.L. Hase, *Chemical Kinetics and Dynamics*, Prentice Hall 1989.

K. J. Laidler, *Chemical Kinetics*, 3rd edition, Harper and Row, 1987.

R. D. Levine and R. B. Bernstein, *Molecular Reaction Dynamics and Chemical Reactivity*, Oxford University Press, 1987.

J. W. Moore and R. G. Pearson, *Kinetics and Mechanisms*, John Wiley and Sons, 1981.

CH 427 Chemical and Statistical Thermodynamics

2 1 0 6

Applications of thermodynamic functions; partial molar quantities; non ideality and activities; chemical equilibria. Ensembles, MB, BE and FD distributions; Partition functions and their relationships to thermodynamic functions and equilibrium constant; Virial coefficients; Lattice Models; Introduction to non-equilibrium thermodynamics; Onsager`s reciprocity relations.

Text / References

P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th edition, Oxford University Press, 2006.

K. S. Forland, T. Forland and S.K. Ratkje, *Irreversible Thermodynamics, Theory and Applications*, John Wiley, 1988.

G. W. Castellan, *Physical Chemistry*, 3rd edition, Narosa Publishing House, 1985

R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, John Wiley, 1980.

F. T. Wall, *Chemical Thermodynamics*, W. H. Freeman and Co., 1965.

G. N. Lewis, M. Randall, K.S. Pitzer and L. Brewer, *Thermodynamics*, McGraw Hill, 1961.

T. L. Hill, *Statistical Thermodynamics*, Addison Wesley, 1960.

D. A. McQuarrie and J. D. Simon, *Physical Chemistry - a molecular approach*, Viva Books Pvt. Ltd. (1998)

CH 429 Modern Methods of Analysis

2 1 0 6

Evaluation of reliability of analytical data and statistics in chemical analysis. Expression of results to significant figures. Sampling and preparation of sample for analysis. Introduction to optical methods, ultraviolet, visible, infrared spectrophotometry and fluorimetry. Atomic absorption and flame emission spectroscopy. Scattering of radiation, nephelometry, turbidimetry and Raman Spectroscopy. Electroanalytical methods such as voltammetry, polarography, amperometry, conductometry and high frequency titrations. Thermogravimetry

and differential thermal analysis. Introduction to interphase separations with special reference to chromatography. Gas chromatography and HPLC.

Text References

G .W. Ewing, Instrumental methods of chemical analysis, 5th Edition, McGraw-Hill, 1985.

H. H. Willard, L. L. Merritt, J. A. Dean and F. A. Settle, Instrumental Methods of Analysis, 6th Edition, Van Nostrand Reinhold, 1980.

H. A. Laitinen and W. A. Harris, Chemical Analysis, 2nd Edition McGraw-Hill, 1975.

CH 432 Inorganic Chemistry Lab III

0 0 4 4

Complexometric titrations by masking and demasking reactions. Estimations by nephelometry, fluorimetry, simultaneous spectrophotometry, atomic absorption spectroscopy. Determination of composition of complexes in solution. Synthesis and characterization of transition metal complexes (including organometallic compounds) and their study by spectral, magnetic and thermal methods.

CH 433 Physical Chemistry Lab II**0 0 4 4**

Phase equilibria, viscosity and molecular weight of polymers, surface tension, reaction kinetics (rates, order of reaction, influence of ionic strength), use of thermocouples, transition temperature determinations, self generated experiment.

CH 434 Physical Chemistry Lab III**0 0 4 4**

Determination of the following physical quantities : partial molal volumes, dipole moments, activities by freezing point, quantum yields, heats of vaporisation and depressions of freezing points of solutions, velocity constant and activation energy. Electrodes with different substrates for H₂ evolution, photoelectrochemical solar cells. Vacuum measurement. IR spectrum of HCl, Use of M.O. theory, solution of Schrodinger equation for polyatomics.

CH 437 Chemistry of Transition Elements**2 1 0 6**

General chemistry of the transition elements, lanthanides and actinides including atomic nuclei and nuclear reactions, coordination chemistry including theories of metal-ligand bonding, spectral and magnetic properties, organometallic compounds of transition elements, role of transition metal ions in biological processes.

Texts/References

F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, Wiley Eastern, John Wiley, 6th edition, 1999.

J. E. Huheey, E. Keiter and R. Keiter, *Inorganic Chemistry*, 4th edition, Harper Collins College Publisher, 1993.

D. Banerjea, *Inorganic Chemistry Principles*, Books Syndicate Pvt. Ltd., 2000

N. N. Greenwood and E. A. Earnshaw, *Chemistry of Elements*, Pergamon Press, 1989

CH 438 Chemistry of Main Group Elements**2 1 0 6**

Chemistry of non-transition elements, stereochemistry and bonding in non-transition elements and compounds. Solvents, solutions, acids and bases, brief review of inorganic chains, rings and

cages, organometallic compounds of non-transition elements, role of non-transition elements in biological processes.

Texts/References

F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, John Wiley, 6th edition, John Wiley, 1999.

C. Elschenbroich and A. Salzer, *Organometallics*, 2nd edition, Wiley VCH, 1992.

D. F. Shriver, P. W. Atkins and C. H. Langford, *Inorganic Chemistry*, Oxford University Press, 3rd edition, 1999.

CH 481: Chemistry and Computers

2026

Numerical computing using a high level language like FORTRAN/C: Programming principles using loops, arrays and functions; use of libraries; Numerical methods: truncation and round off errors; roots; interpolation; differentiation and integration; linear equations, matrix operations; curve fitting; ODEs; optimization; Application of numerical methods to chemical problems.

Text/References

S. J. Chapman, *Fortran 90/95 for Scientists and Engineers*, 2nd edition, McGraw-Hill, 2003.

W. E. Mayo and M. Cwiakala, *Programming with FORTRAN 77, Schaum's Outline Series*, McGraw Hill, 1995.

A. Kelly and I. Pohl, *A book on C* 4th edition, Addison-Wesley, 1999.

S. C. Chapra and P. Canale, *Numerical Methods for Engineers* 4th edition, Tata McGraw-Hill , 2002.

R. J. Schilling and S. L. Harris, *Applied Numerical Methods for Engineers: Using MATLAB and C*, Brooks/Cole Publishing Company <<http://www.brookscole.com>>, 2000.

J. H. Mathews, *Numerical Methods for Mathematics, Science, and Engineering* 2nd edition, Prentice Hall of India, 2001.

CH 502 Synthesis and characterization of Inorganic Compounds.**2 1 0 6**

Preparative chemistry of compounds of main group and transition elements including inorganic chains, rings, cages, clusters, halogen and rare gas compounds. Experimental problems encountered in the synthesis, isolation, purification, characterization and identification of inorganic compounds. Physical methods for characterization, PES, EXAFS, Mossbauer spectroscopy, magnetic susceptibility and cyclic voltammetry.

Text/References

R. S. Drago, *Physical Methods for Chemists*, Saunders, 1992.

R. J. Angelias, *Synthesis and Techniques in Inorganic Chemistry*, 2nd edition, Saunders, 1977.

G. Pass and H. Sutchliffe, *Practical Inorganic Chemistry: Preparation, Reactions and Instrumental Methods*, 2nd edition, Chapman and Hall, 1974.

W. L. Jolly, *The Synthesis and Characterization of Inorganic Compounds*, Prentice Hall, 1970.

CH 504 Computational Chemistry**1 0 4 6**

A brief outline of molecular mechanics, semi-empirical approximations, ab initio methods, basis sets and Z-matrix; Application of these computational methods for prediction of structural and electronic properties of molecules by using standard programs; FMOs in organic chemistry, crystal and ligand field calculations, computation of potential energy surfaces. Conformational analysis by molecular mechanics; Dynamical and structural studies of molecules using molecular dynamics simulations; Monte Carlo simulations of molecules.

Texts/References:

C. J. Cramer, *Essentials of Computational Chemistry: Theories and Models*, John Wiley & Sons, 2002.

D. Young, *Computational Chemistry: A practical Guide for applying Techniques to Real World Problems*, Wiley Interscience, 2001.

A. R. Leach, *Molecular Modelling: Principles and Applications*, Pearson Education, 2001.

J. B. Foresman, A. Frisch, *Exploring Chemistry with Electronic Structure Methods*. Gaussian Inc., 1996.

M. P. Allen and D. J. Tildesley, *Computer Simulations of Liquids*, Oxford, 1987

CH 507 Methods in Organic Synthesis**2 1 0 6**A
revie
w of

various synthetic methods in organic chemistry: Formation of C-C, C=C, C≡C bonds and various rings (namely 3, 4, 5, 6, 7 and 8-membered ring) with special emphasis on utility of several types of organometallic reagents. Selected syntheses of natural and unnatural products having these ring systems. A concise introduction to various aspects of asymmetric synthesis followed by detailed discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts, and organocatalysts with specific examples. A brief discussion on biosynthesis and biomimetic synthesis with selected examples from monoterpenes, sesquiterpenes, diterpenes, steroids, and alkaloids. Introduction of domino and tandem reaction concepts with a detailed discussion on selected examples.

Texts/References:

G. S. Zweifel and M. H. Nantz, *Modern Organic Synthesis-An Introduction*, W. H. Freeman and Company, 2006

F. A. Carey, R. Sundberg, *Advanced Organic Chemistry, Part B*, 5th edition, Plenum Press, 2007.

R. O. C. Norman and J. M. Coxon *Principles of Organic Synthesis* 3rd edition, Nelson Thornes, 2005.

M. B. Smith and J. March, *March's Advanced Organic Chemistry*, 5th edition, Wiley, 2001.

B. M. Trost and I. Fleming, *Comprehensive Organic Synthesis*, Pergamon Press, 1992

CH-508 Bioorganic chemistry**2 1 0 6**

General comparison of organic reactions carried out in laboratory and organic reactions observed in biological systems. Nature of biomolecular interactions, physical concepts. Stereospecificity and rate enhancement in enzyme catalysed reactions. Discussion on non-availability of electrophilic sites in enzymes and their presence in co-enzymes. Following reactions will be discussed (comparing the usual mechanism to enzyme catalysed mechanism) : hydrolysis of esters, amides, phosphoesters, etc. C-C and C=C bond formation, oxidation, reduction and decarboxylation. Remote functionalisation cyclisation reactions. Biomimetic reactions. Hydrophobicity, organized assemblies. Supramolecular structure, drug design.

Text/References

Bioorganic Chemistry Frontiers Vol.2, Ed. H. Dugas, Springer-Verlag, pp.1-252, 1990.

H. Dugas, *Bioorganic Chemistry. A Chemical approach to enzyme action*, 2nd Edn., Springer-Verlag, 1989.

D. E. Metzler, *Biochemistry-The Chemical Reactions of a Living Cell*, Academic Press, 1977.

E. E. Tamlen, *Bioorganic Chemistry*, Academic Press, 1977.

CH 510 Heterocyclic chemistry

2 1 0 6

Introduction to heterocyclics and their importance. Nomenclature of ring systems, structure, reactivity and synthesis of reduced three, four, five and six membered oxygen, nitrogen and sulphur heterocyclics; aromatic heterocyclics, 5-membered, 6-membered and polyhetero ring systems - indole, azoles and diazines. Constitution and configuration of simple sugars, chemical reactions of monosaccharides and their cyclic anomers.

Texts/References

R. K. Bansal, *Heterocyclic Chemistry, Synthesis, Reactions and Mechanisms*, Wiley Eastern Ltd., 1990.

J. A. J. Joule and G. F. Smith, *Heterocyclic Chemistry*, ELBS, 2nd edition, 1982.

F.G. Riddell, *The Conformational Analysis of Heterocyclic Compounds*, Academic Press, 1980.

L.A. Paquette, *Principles of Modern Heterocyclic Chemistry*, W.B. Benjamin, Inc., 1978.

B.M. Acheson, *An Introduction to the Chemistry of Heterocyclic Compounds*, Interscience, 2nd edition 1975.

CH 521 Interpretative Molecular Spectroscopy

2 1 0 6

Mass spectrometry, the production and analysis of positive ions, molecular ions, application of isotopic abundance measurements, fragmentation modes and rearrangement of ions. Mass spectra of certain chemical classes. Electronic spectroscopy (UV-visible, fluorescence and phosphorescence): Simple chromophoric groups, conjugated and aromatic systems. Characteristic absorption of organic and inorganic compounds. Infrared spectroscopy: Characteristic group frequencies of organic and inorganic molecules. Nuclear magnetic resonance spectroscopy of compounds containing ^1H , ^{13}C , ^{19}F and ^{31}P nuclei. Identification of organic and inorganic compounds using combination of spectral data.

Text/References

R. S. Drago, *Physical Methods for Chemists*, W. B. Saunders, 1992.

R. M. Silverstein, C. G. Bassler and T. C. Morrill, *Spectrophotometric Identification of Organic Compounds*, 5th edition, Wiley, 1991.

D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 3rd edition, McGraw Hill, 1980.

W. Kemp, *Organic Spectroscopy*, ELBS, 1979.

W. L. Jolly, *The synthesis and characterization of inorganic compounds*, Prentice-Hall, 1970.

CH 522 Chemistry of Coordination compounds

2 1 0 6

Classification of ligands by donor atoms, stability, reactivity, bond types, geometry and coordination compounds. Kinetics and mechanism of reactions of transition metal complexes : substitution reactions, electron transfer redox processes, acid base and related processes. Inorganic photochemistry of coordination compounds.

Text/References

F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th edition, Wiley, 1999

J. E. Huheey, E. Keiter and R. Keiter, *Inorganic Chemistry*, 4th edition, Harper Collins College Publisher, 1993.

R. G. Wilkins, *Kinetics and Reaction Mechanism of Transition Metal complexes*, 2nd revised edition, VCH, New York, 1991.

F. Basolo and R.G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edition, Wiley, 1967.

CH-523 Molecular Spectroscopy

2 1 0 6

Introduction to spectral energy domains and measurement of spectra, Implications of discrete energy levels, Population of States – Boltzman Distribution, Interaction of radiation with matter, origin of linewidths in molecular spectra, Transition dipole moment and Fermi's Golden Rule, Einsteins Coefficients, Lasers and Masers;

Rotational (Microwave) spectroscopy, Molecular vibrations - Infrared spectroscopy, Normal mode analysis, Raman Scattering, Selection Rules from Group Theory, Molecular electronic spectra, Photophysical processes, Non-Linear Spectroscopy, Nuclear Magnetic Resonance, Relaxation times, FT-NMR, spin-spin coupling, ESR, Nuclear Quadrupolar Resonance.

Text/References

J. L. McHale, *Molecular Spectroscopy*, Pearson Education, 1999.

- M. Hollas, *Modern Spectroscopy*, Wiley; 4th edition, 2004.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3rd edition, Wiley-Interscience, 1990.
- D. C. Harris, M. D. Bertolucci, *Symmetry and Spectroscopy*, Dover, 1990.
- C. M. Banwell, E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw Hill, 1983
- G. M. Barrow, *Molecular Spectroscopy*, McGraw Hill, 1962
- J. I. Steinfeld, *Molecules and Radiation: An Introduction to Modern Molecular Spectroscopy*, 2nd edition, Dover, 2005.
- J. D. Graybeal, *Molecular Spectroscopy*, McGraw Hill 1993.
- D. A. McQuarrie and J. D. Simon, *Physical Chemistry - a molecular approach*, Viva Books Pvt. Ltd. 1998.

CH-524 Bioinorganic Chemistry

2 1 0 6

Chemical make up and essential inorganic elements of organisms. Chemistry aspects of metal complexes. Spectral, biochemical and biological methods used in bioinorganic chemistry. Bioinorganic chemistry of Na⁺, K⁺, Mg²⁺ and Ca²⁺. Role of metal ions in biology: Proteins and enzymes of V, Mn, Fe, Co, Ni, Cu, Zn and Mo. Structural and functional models. Transport and storage of metal ions. Carcinogenicity of chromium. Selenium in biology.

Text/References

- S. J. Lippard and J. M. Berg, *Principles of bioinorganic chemistry*, University Science Books, Mill Valley, 1994.
- I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Univ. Sci. Books, Mill Valley, 1994.
- J. A. Cowan, *Inorganic Biochemistry*, VCH Publishers, 1993.
- J. Reedijk, *Bioorganic Catalysis*, Marcel Dekker, Inc. (Ed.), 1993.
- R. W. Hay, *Bioinorganic Chemistry*, Ellis Hollwood, Ltd. 1984.

CH 528 Natural Products

2 1 0 6

Terpenoids : Classification, structure, chemistry and biogenesis of some important mono; sesqui, di, and triterpenes.

Steroids : Sterols and bile acids, estrogens, androgens, gestagens and adrenocortical hormones. Hormone production. Cardiac glycosides. Steroidal triterpenes; biogenesis of steroids and correlation with terpenoids.

Alkaloids : Characteristic reactions, general methods of degradation, structure and chemistry of some well-known alkaloids.

Natural Pigments: Flavones, flavanones, isoflavones, xanthenes, quinones, pterins, chlorophyll and haemin.

Carbohydrates: Stereochemistry, reaction and conformation of monosaccharides, deoxy and aminosugars, hexonic acid and vitamin C, disaccharides, polysaccharides, inositol; gangliosides and other glycosides. Chemistry of vitamins A,B,C and E.

Text/References

I. L. Finar, *Organic Chemistry, Vol .2*, 5th edition, ELBS, 1975.

K. Nakanishi, T. Goto, S.Ito, S. Najori and S. Nozoe, *Natural products Chemistry, Vol. 1 and 2*, Academic Press, 1974.

A. A. Newman, *Chemistry of Terpenes and Terpenoids*, Academic Press, 1972.

S. W. Pelletier, *Chemistry of the Alkaloids*, Van Nostrand Reinhold, 1970.

C. W.Shoppee, *Chemistry of the Steroids*, 2nd edition, Butter worths, 1964.

R. D. Guthrie and J. Honeyman, *An Introduction to the Chemistry of Carbohydrates*, 3rd edition, Clarendon Press, 1968.

T. A. Geissman, *Chemistry of Flavonoid Compounds*, Pergamomn Press, 1962.

CH 540 Drugs and Biologically Active Compounds

2 1 0 6

Drug receptor interactions. Approaches to drug design. Drug metabolism. A few drugs from each of the following groups will be discussed.

Analgesics, antidepressants, antipsychotics, antiinflammatory agents, cardiovascular agents, diuretics, antibacterials, antibiotics, antivirals, antimalarials, antiamebics, drugs for neoplastic diseases.

Vitamins : A, B1, B2, B6 niacin, folic acid, dantothenic acid, biotin, B12,C,D,E and K. Hormones : Thyroid hormones and antithyroid drugs. Steroid hormones and some important steroidal drugs.

Texts/References

A. Burger, *Medicinal Chemistry*, 4th edition, Wiley Interscience, 1981.

R. F. Doerge, Ed., *Wilson and Gisvold's Text Book of Organic Medicinal and Pharmaceutical chemistry*, 8th edition, J. B. Lippincott Co., 1982.

D. Lednicer and L. A. Mitscher, *The Organic Chemistry of Drug Synthesis*, Wiley Interscience, 1977.

O. L. Salerini, *Natural and Synthetic Organic Medicinal Compounds*, C. V. Mosby Co., 1976.

CH 546 Introduction to Biomolecules

2 1 0 6

Molecular logic of living matter. Origin of biomolecules. Cell structure. Amino acids structure, functional group properties and reactions. Protein structure, conformation and biomolecular interactions. Sugar-polysaccharides, structure and functions. Nucleotides, nucleic acids structure and function, DNA organisation, replication, transcription, ribosomes, genetic code and protein synthesis. Enzymes-categorization, catalysis, kinetics-single substrate enzyme catalyzed reactions, inhibition. Lipids-structure and properties of different classes of lipids. Biomembrane organisation-membrane lipids. Membrane bound proteins-structure, properties and transport phenomena. Bioenergetics-basic principles, glycolytic pathways, Krebs's cycle, oxidative phosphorylation, coupled processes. Photosynthesis.

Texts/References

J. M. Berg, J. L. Tymoczko, L. Stryer, *Biochemistry*, International Edition, W. H. Freeman and Company, 2006.

A. Lehninger, D. L. Nelson, M. M. Cox, *Principles of Biochemistry*, 5th edition, W. H. Freeman and Company, 2008.

G. M. Blackburn, M. J. Gait, D. Loakes, D. M. Williams, *Nucleic Acid in Chemistry and Biology*, 3rd edition, RSC Publishing, London 2006.

V. Voet and J. G. Voet, *Biochemistry*, John Wiley, New York, 2004.

R. J. Simond, *Chemistry of Biomolecules*, Royal Society of Chemistry, U.K. London, 1992.

CH-547 Organometallic Chemistry

2 1 0 6

Historical background, factors controlling metal-carbon bond formation, methods of M-C bond formation, comparative survey of structure and bonding of metal alkyls and aryls, complexes with p acids, CO and related ligands, complexes with olefins, acetylenes and related unsaturated molecules, catalytic properties of mononuclear compounds, stereochemical non-rigidity in organometallic compounds, boranes, carboranes and metallocarboranes, bimetallic and cluster complexes, structure and applications in catalysis, applications of organometallic

compounds in organic synthesis, enantioselective synthesis via organometallic compounds, importance of organometallic compounds in certain biological systems.

Text/references

G. O. Spessard, G. L. Miessler, *Organometallic Chemistry*, Prentice Hall, 1997.

C. Elsehenbroich and A. Salzer, *Organometallic Chemistry*, 2nd edition, Wiley VCH, 1992.

F. A. Cotton, G. Wilkinson, C. A. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th edition, Wiley, 1999.

N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 1st edition, Pergamon, 1985.

B. F. G. Johnson, *Transition Metal Clusters*, Wiley, 1980.

G. Wilkinson, F. G. A. Stone and E. Abel, *Comprehensive Organometallic chemistry*, Pergamon, 1980.

CH 550 Electrochemistry

2 1 0 6

Nernst equation. Origin of EMF of a galvanic cell. Polarizable and non-polarizable electrodes, the electrocapillary curve, null point of metals and its determination. Thermodynamics of electrical double layer, Lipmann equation, measurement of surface excess. Models for the electrical double layer. Electrode kinetics. The concept of over potential. Electrochemical reactions under mass transfer control, chronopotentiometry, voltammetry and polarography. Electrochemical reactions under charge transfer control, generalized Butler Volmer equation, determination of kinetic parameters. Mechanism and electrocatalysis of hydrogen and oxygen evolution reactions.

Text/References

D. I. Antropov, *Theoretical Electrochemistry*, Mir Publishers, 1972.

J. Koryta, J. Dvorak, V. Bohackova, *Electrochemistry*, Methuen & Co. Ltd., 1970.

J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry, Vol.1 and 2*, Plenum Press, 1998.

Adsorption isotherms: Langmuir, BET, Frumkin, Temkin and Freundlich. Adsorption on porous solids. Chemisorption of gases on metals and semiconductors. Kinetics of adsorption processes, heterogeneous catalysis. Catalysis by metals, semiconductors and solid acids. Characterization of solid surface structure and composition using electron microscopy, FEM, XPS, Auger, Mossbauer, SIMS, ISS and LEED.

Text/References

- D. K. Chakrabarty, *Adsorption and catalysis by solids*, Wiley Eastern, 1990.
F. P. Kane and G. B. Larrabee (Eds.), *Characterisation of solid surfaces*, Plenum, 1978.
A. W. Adamson, *Physical Chemistry of Surfaces*, 3rd edition, Wiley Interscience, 1976.
A. Clark, *The Theory of Adsorption and Catalysis*, Academic Press, 1970.

Introduction and applications of polymers, molecular weight distributions, various experimental methods (GPC/SEC, solution viscosity, VPO, light scattering) to determine relative and absolute molecular weight distributions, chain growth and step growth mechanisms and kinetics, ionic polymerization, living polymerization, stereochemistry of polymers, free radical copolymerization (random, block, alternate and graft copolymers), kinetics and mechanisms of free radical copolymerization, polymerization conditions and polymer reactions, thermal, mechanical and solution properties of polymers, thermoplastics, thermosets and elastomers, conducting polymers, branched polymers (star, dendritic and hyperbranched polymers).

Text/References

- G. Odian, *Principle of Polymerization* 3rd edition, John Wiley, 1991
P. J. Flory, *Principles of Polymer Chemistry*, Cornell University Press, 1953
M. Chanda, *Advanced polymer chemistry: a problem solving guide*, Marcel Dekker, 2000
F. W. Billmeyer Jr., *Textbook of Polymer Science* 3rd edition, John Wiley, 1991

Structure of solids, surfaces, interfaces and soft matter, electronic structures, structure and properties of nanocrystals. Introduction to polymers; physical properties of polymers; classification of polymers based on kinetics and methods to characterize polymers. Structural Inorganic Chemistry: Basic aspects of single crystal X-ray diffraction, methods of structure determination and interpretation of structures.

Homogeneous catalysis: Metal ions in organic transformation, basic principles, activation energy, essential steps in catalysis, catalytic transformation to useful organic compounds.

Text/References

P. A. Cox, *Electronic Structure and Chemistry of Solids*, Oxford University Press, 1991.

G. Odian, *Principle of Polymerization* 3rd edition, John Wiley, 1991

P. J. Flory, *Principles of Polymer Chemistry*, Cornell University Press, 1953

M. Chanda, *Advanced polymer chemistry: a problem solving guide*, Marcel Dekker, 2000

F. W. Billmeyer Jr., *Textbook of Polymer Science* 3rd edition, John Wiley, 1991

G.H. Stout and L.H. Jensen, *X-ray Structure Determination: A Practical Guide*, 2nd edition, John Wiley, 1989.

Ch. Elschenbroich, *Organometallics*, 3rd edition, Wiley-VCH: Weinheim, 2006.

P.W. van Leeuwen, *Homogeneous Catalysis: Understanding the art*, Kluwer, 2005.

CH 559 Solid State Chemistry and Its Applications

2 1 0 6

Diffraction techniques and the structure of solids; analysis of diffraction data. Crystal defects, nonstoichiometry and solid solutions. Structure of solid electrolytes, zeolites, conducting polymers and surfaces. Solid state transformations and reactions.

Electronic structure of solids: Fermi level, Bloch orbitals, energy bands, Brillouin zone. Electric and magnetic properties of solids: insulators, semiconductors, conductors and Fermi surfaces; superconductivity; polarization, refractive index, dielectrics and ferroelectrics; diamagnetism and paramagnetism; ferromagnetism, ferrimagnetism and antiferromagnetism. Molecular metals, phosphors and solid state lasers.

Texts/References

C. Kittel, *Introduction to Solid State Physics*, 6th edition, Wiley, 1991.

A. R. West, *Solid State Chemistry and Its Applications*, Wiley, 1989.

P. A. Cox, *Electronic Structure and Chemistry of Solids*, Oxford University Press, 1991.

A. W. Adamson, *Physical Chemistry of Surfaces*, Wiley, 1990.

H. V. Keer, *Principles of the Solid State*, Wiley Eastern, 1993.

D. K. Chakrabarty, *Solid State Chemistry*, New Age International, 1996.

A. Zangwill, *Physics at Surfaces*, Oxford University Press, 1988.

CH 560 Quantum Chemistry

2 1 0 6

Matrix formulation of quantum mechanics: transformation, representations, projection operators, equations of motion. Operator formalism: Virial theorem, normal operators, Dirac's method of solution of harmonic oscillator problem. Angular momentum: ladder operator technique, solutions, differential equation methods, spin, addition of angular momenta. Explicit derivation of Hartree and Hartree-Fock equations, Roothaan equations, basis sets - STO and GTO, calculation of integrals, semiempirical methods. Configuration interaction. Tunnel effect: square barrier, WKB approximation, electron and proton transfer. Many-body treatments: correlation energy, N-dependence, diagrammatic representations and linked cluster theorem.

Texts/References

I. R. Levine, *Quantum Chemistry*, Prentice Hall India (Ltd.), 1995.

A. Szabo and N. S. Ostlund, *Modern Quantum Chemistry*, McGraw-Hill, 1989.

J. Goodisman, *Contemporary Quantum Chemistry*, Plenum, 1977.

F. L. Pilar, *Elementary Quantum Chemistry*, McGraw-Hill, 1968.

S. N. Datta, *Lectures on Chemical Bonding and Quantum Chemistry*, Prism Books, 1998.

CH-574 Topics in Inorganic Chemistry-I

2 1 0 6

Electron transfer properties of metal complexes. Molecular recognition. Asymmetric catalysis. Phosphorus compounds as ligands. Cluster chemistry. Bio-inorganic reaction mechanisms.

Text/References

W. L. Jolly, *Modern Inorganic Chemistry*, McGraw, Hill Co., 1984.

R. W. Hay, *Bioinorganic Chemistry*, Wiley, 1984.

M. Day and J. Selbin, *Theoretical Inorganic Chemistry*, 2nd edition, Von. Nostrand, 1980.
H. J. Emeleus and J. J. Anderson, *Modern Aspects of Inorganic Chemistry*, Von. Nostrand, 1962.

CH-576 Statistical Mechanics

2 1 0 6

Ensembles and Averages, equivalence of Ensembles, classical Limit. Monte Carlo and Molecular Dynamics simulations. Distribution functions at equilibrium. Integral equation methods. Perturbation theory. Density functional methods. Molecular fluids. Estimation of thermodynamic functions. Non-equilibrium methods. Linear response theory. Projection operator method. Stochastic processes and Brownian motion. Selected applications to problems in chemical dynamics, relaxation processes and neutron diffraction.

Texts/References

M. P. Allen and D. J. Tildesley, *Computer Simulation in Liquids*, Oxford University Press, 1987.

J. P. Hansen and I. R. McDonald, *Theory of Liquids*, 2nd edition, Academic Press, 1986.

D. Chandler, *Statistical Mechanics*, Oxford University Press, 1985.

H. L. Friedman, *A Course in Statistical Mechanics*, Prentice Hall, 1983.

L. D. Landau, E. M. Lifshitz and L. P. Pitaevskii, *Statistical Physics Parts I and II*, Pergamon Press, 1980

D. A. McQuarrie, *Statistical Mechanics*, Harper and Row, 1974.

CH-578 Topics in Inorganic Chemistry - II

2 1 0 6

Basic aspects of single crystal diffraction. Molecular metals. Inorganic rings. Transition metal chemistry of macrocycles. Metal ions in medicine. Fluxional molecules.

Text/References

J. E. Huheey, *Inorganic Chemistry*, 4th edition, Harper Collins College Publisher, 1993.

G. H. Stout and L. H. Jensen, *X-ray Structure Determination : A Practical guide*, 2nd edition, John Wiley, 1989.

J. P. Ferraro and J. M. Williams : *Introduction to synthetic electrical conductors*, Academic Press, 1987.

- B. Sarkar (Ed.), *Biological Aspects of Metals related Diseases*, Raven Press, 1983.
- G. A. Melson (Ed.), *Coordination Chemistry of Macrocyclic Compounds*, Plenum Press, 1979.
- D. E. C. Corbridge, *The Structural Chemistry of Phosphorus*, Elsevier, 1974.

CH 582 Inorganic Photochemistry

2 1 0 6

Introduction to inorganic photochemistry. Photochemical laws and photochemical kinetics. Photophysical processes. The electronic absorption spectra of inorganic compounds. Characteristics of the electronically excited states of inorganic compounds. Photoelectrochemistry of excited state redox reactions. Photosensitization. Photochemical reactions; substitution, decomposition and fragmentation, rearrangement, and redox reactions. Selective inorganic photochemistry using laser beams. Inorganic photochemistry in biological processes and their model studies.

Text/References

- G. L. Geoffrey and M. S. Wrighton, *Organometallic Photochemistry*, Academic Press, 1979.
- K. K. Rohatagi-Mukherjee, *Fundamentals of Photochemistry*, Wiley Eastern, 1978.
- M. S. Wrighton, *Inorganic and Organometallic Photochemistry*, ACS Pub., 1978.
- V. Balzani and V. Carasiti, *Photochemistry of Co-ordination compounds*, Academic Press, 1970.

CH-584 Biophysical Chemistry

2 1 0 6

Structure of water. Biological relevance of chemical potential. Hydrophobic and hydrophilic interactions in biological systems. Protein-Solvent Interactions - preferential binding, hydration and exclusion. Protein structure, stability, folding, unfolding and their studies with spectroscopic and calorimetric methods. Protein-Ligand Binding. Structure-Function relationships. Equilibria across membranes.

Text/References

- R. B. Gregory, ed., *Protein-Solvent Interactions*, Marcel Dekker, Inc., 1995.
- B. T. Nall and K. A. Dill, ed., *Conformations and Forces in Protein Folding*, American Association for the Advancement of Science, 1991.

C. Branden and J. Tooze, *Introduction to Protein Structure*, Garland Publishing, Inc., 1991.

J. Wyman and S. J. Gill, *Binding and Linkage : Functional Chemistry of Biological Macromolecules*, University Sciences Books, 1990.

C. R. Cantor and P. R. Schimmel, *Biophysical Chemistry, Part III*, W.H. Freeman and Co., 1980.

CH 586 Structure and Properties of Materials

2 1 0 6

Common structure of elements and compounds. Bonding in solids. Structure determination by X-ray diffraction methods. Diffusion in solids. Electrical, magnetic, optical, dielectric and thermal properties of solids.

Text/References

H. V. Keer, *Principles of the Solid State*, Wiley Eastern Ltd., 1993.

C. Kittel, *Introduction to Solid State Physics*, John Wiley & Sons, 1991.

A. R. West, *Solid State Chemistry and Its Applications*, John Wiley & Sons, 1989.

A. F. Wells, *Structural Inorganic Chemistry*, Clarendon Press, 1986.

L. V. Azaroff, *Elements of X-ray Crystallography*, McGraw-Hill, 1968.

CH 588 Organic Synthesis

2 1 0 6

Concepts of symmetrization, umpolung, selectivity and specificity (stereo, regio and chemo). Antithetic and metathetic approaches. Selective introduction and manipulation of functional groups. Selectivity in functional groups reactions, activation, protection and blocking of groups. C-C bond forming reactions-cyanohydrin formation, organometallic additions, Wittig and related reactions, halomethane addition, nucleophilic substitution, Aldol condensation, enolate alkylation, Friedel-Crafts reaction, Michael reaction, Claisen condensation, Cope and Claisen rearrangements, inter- and intra molecular Diel's-Alder reactions, Barbier Weiland degradation, Dieckmann and acyloin condensations, directed aldol condensation, conjugate addition and annulation reactions. Photochemical synthesis. Applications of the above methodologies in the synthesis of key synthones and other molecules.

Text/References

S. Warren, *Designing Organic Synthesis*, John Wiley and Sons, 1980.

W. Caruthers, *Some Methods of Organic Synthesis*, Cambridge University Press, 1978.

H. O. House, *Modern Synthetic Reactions*, 2nd Ed., W.A.Benjamin 1972.

R.O.C. Norman, *Principles of Organic Synthesis*, 2nd Edn., Methuen and Co. Ltd., 1972.

CH 5XY Macromolecular Crystallography

2 1 0 6

Basic Diffraction Theory, Bragg's law, Miller Indices, Laue Equations, Protein and Nucleic acid Structure, X-ray major sources and production, Xray detectors, Crystallization techniques and principles, symmetry and space groups, reciprocal space, Fourier transform, structure factor equation, phase problem, data collection and processing, methods of structure determination, heavy atom solutions like direct methods, patterson methods, Multiple Anomalous diffraction, Single Anomalous diffraction, sulphur phasing, Isomorphous replacement, Molecular replacement, structure refinement and validation, structure deposition, elucidation of mechanism from structure, biological crystallography examples of virus, ribosomes, membrane proteins, macromolecular assemblies

Suggested Text:

[Principles of protein x-ray crystallography](#) Jan Drenth,

Crystallography Made Crystal Clear , Gale Rodes

[Structure determination by X-ray crystallography](#) M. Ladd and R Palmer

CH-593 : M. Sc. Project

12

CH-594 : Project

18