Four Year Bachelor of Science programme

Department of Chemistry
Indian Institute of Technology Bombay

Academic Curricula

CURRICULUM FOR 4 YEAR B. S. PROGRAMME

First year : First Semester

In accordance with Institute curriculum

First year : Second Semester

In accordance with Institute curriculum, with the following DIC:

Code	Name	L	T	P	C
CH 10x	Chemistry-II	2.0	1.0	0.0	6.0

Second year : First Semester

Code	Name	L	T	P	C
CH 210	Introduction to transition metal chemistry	2.0	1.0	0.0	6.0
CH 211	Chemical thermodynamics	2.0	1.0	0.0	6.0
CH 22A	Structure and Stereochemistry	2.0	1.0	0.0	6.0
HS 101	Economics	2.0	1.0	0.0	6.0
CH 2XY	Data analysis for Chemists	2.0	1.0	0.0	6.0
CH 206	Inorganic Chemistry Lab -I	1.0	0.0	3.0	4.0
		11.0	5.0	3.0	34.0

Contact hours: 19.0
Credits: 34.0

Second year : Second Semester

Code	Name	L	T	P	C
CH 222	Reactions of carbonyl compounds	2.0	1.0	0.0	6.0
IE1	Institute Elective from HSS	2.0	1.0	4.0	6.0
CH 2BC	Co-ordination chemistry	2.0	1.0	0.0	6.0
ES 200/	Environmental science and engineering/	3.0	0.0	0.0	3.0
HS 200	Environmental studies	3.0	0.0	0.0	3.0
	(Half-semester courses)				
CH 215	Physical Chemistry Lab - I	0.0	0.0	4.0	4.0
CH 218	Organic Chemistry Lab- I	0.0	0.0	4.0	4.0
		9.0	3.0	12.0	32.0

Contact hours: 24.0
Credits: 32.0

Third year : First Semester

Code	Name	L	T	P	C
CH 423	Organic Reactions	2.0	1.0	0.0	6.0
CH ABC	Electrochemistry of Solutions and Interfaces	2.0	1.0	0.0	6.0
CH 425	Chemical Bond and Molecular Geometry	2.0	1.0	0.0	6.0
CH 437	Advanced Transition metal chemistry	2.0	1.0	0.0	6.0
CH 4AB	Inorganic Chemistry Lab - II	0.0	0.0	4.0	4.0
CH 433	Physical Chemistry Lab - II	0.0	0.0	4.0	4.0
CH 4KP	Organic Chemistry Lab-II	0.0	0.0	4.0	4.0
		8.0	4.0	12.0	36.0

Contact hours: 24.0
Credits: 36.0

Third year : Second Semester

Code	Name	L	T	P	C
CH 416	Physical Organic Chemistry/ (Half semester)	2.0	1.0	0.0	3.0
CH 4GP	Thermal and Photochemical reactions (Half semester)	2.0	1.0	0.0	3.0
CH 442	Molecular Spectroscopy	2.0	1.0	0.0	6.0
CH 4$$	Molecular Energetics and Dynamics	2.0	1.0	0.0	6.0
CH 438	Main Group Chemistry	2.0	1.0	0.0	6.0
CH 418	Organic Chemistry Lab – III	0.0	0.0	4.0	4.0
CH 432	Inorganic Chemistry Lab - III	0.0	0.0	4.0	4.0
CH 434	Physical Chemistry Lab - III	0.0	0.0	4.0	4.0
		8.0	4.0	12.0	36.0

Contact hours: 24.0
Credits: 36.0

Fourth year : First Semester

Code	Name	L	T	P	C
CH 521	Interpretative Molecular Spectroscopy	2.0	1.0	0.0	6.0
CH 546	Bioorganic Chemistry	2.0	1.0	0.0	6.0
CH 547	Organometallic Chemistry and Catalysis	2.0	1.0	0.0	6.0
IE2	Institute Elective II	2.0	1.0	0.0	6.0
CH GHI	Research Project I				6.0
		8.0	4.0	0.0	30.0

Contact hours: 12.0
Credits: 30.0

Fourth year : Second Semester

Code	Name	L	T	P	C
CH EL1	Departmental Elective-I	2.0	1.0	0.0	6.0
CH EL2	Departmental Elective-II	2.0	1.0	0.0	6.0
CH EL3	Departmental Elective-III	2.0	1.0	0.0	6.0
IE3	Institute Elective III	2.0	1.0	0.0	6.0
CH JKL	Research Project II				6.0
		8.0	4.0	0.0	30.0

Contact hours: 12.0
Credits: 36.0

Additional requirement for B. S. (Hons.)

Any four of the following:

		L T P C
CH 584	Biophysical Chemistry	2 1 0 6
CH 4CP	Bioinorganic Chemistry	2 1 0 6
CH 507	Methods in Organic Synthesis	2 1 0 6
CH EL4	Departmental Elective-IV	2 1 0 6
CH GHJ	Mini Project I*	6
CH GHJ	Mini Project II*	6

Total additional credit requirement = 24

**Should be undertaken in 3rd year, 1st and 2nd semesters*

Curriculum for M. Sc. programme after B. S.

Fifth year : First Semester

Code	Name	L	T	P	C
CH EL1	Departmental Elective 1	2.0	1.0	0.0	6.0
CH EL2	Departmental Elective 2	2.0	1.0	0.0	6.0
CH GHI	M. Sc. Project I				30.0
		4.0	2.0	0.0	42.0

Contact hours: 6.0
Credits: 42.0

Fifth year : Second Semester

Code	Name	L	T	P	C
CH EL3	Departmental Elective 3	2.0	1.0	0.0	6.0
CH EL4	Departmental Elective 4	2.0	1.0	0.0	6.0
CH JKL	M. Sc. Project II				30.0
		4.0	2.0	0.0	42.0

Contact hours: 6.0
Credits: 42.0

Departmental electives for B. S. / B. S. + M. Sc. Dual Degree Students

1st Semester

CH 510	Heterocyclic chemistry
CH 582	Inorganic Photochemistry
CH 5ZX	Macromolecular Crystallography

2nd Semester

Physical Chemistry

CH 559	Solid State Chemistry and its Applications
CH 550	Electrochemistry
CH 560	Quantum Chemistry
CH 576	Statistical Mechanics
CH 504	Computational Chemistry

Organic Chemistry

CH 504	Computational Chemistry
CH 528	Natural Products
CH 540	Medicinal Chemistry
CH 556	Polymer Chemistry
CH 588	Organic Synthesis

Inorganic Chemistry

CH 574	Topics in Inorganic Chemistry-I
CH 578	Topics in Inorganic Chemistry-II
CH 5IC	Advanced Co-ordination Chemistry
CH 5XR	X-ray Crystallography

COURSE DETAILS

CH 2XY Data Processing for Chemists

Evaluation of reliability of analytical data and statistics in Chemical Analysis; Statistics of data sampling and dependence on size; Accuracy and Precision; Systematic & Random Errors; Expression of results to significant figures; Error propagation; Standard Deviation and concepts of ESDs; Handling coordinates to yield distances and other metric data; Least Square analysis – curve fitting; Solubility products, Equilibrium and binding/association constants; Sampling and preparation of samples for analyses.

Main Text book
Analytical Chemistry by Gary D. Christian, Wiley-India Edition (6^{th} Ed.) 2004.

CH 206 Principles of Chemical Analysis, Inorganic Chemistry Lab-I 1 0 3 4

Basic concepts of quantitative analysis, methods of sampling, errors in chemical analysis of data, general theory of neutralisation, redox, precipitation and complexometric titrations. Solubility product and precipitation, organic precipitants and extractants. A brief survey of separation methods: solvent extraction and chromatography.
Inorganic Semi-micro qualitative analysis involving 4 radicals. Volumetric analysis involving redox, precipitation and complexometric titrations. Gravimetric estimation of metals. Analysis of alloys and minerals.

Text / References
D. A. Skoog, D. M. West and F. J. Holler, *Analytical Chemistry: An introduction,* 6^{th} edition, Saunders College Publisher, 1994.
G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5^{th} edition, ELBS, 1991.

CH 210 Introduction to transition metal chemistry

Introductory survey of transition elements with reference to electronic configuration, oxidation states, complex compounds. Introductory concepts of molecular symmetry. Spectral and magnetic properties. Introduction to theories of metal-ligand bonding and stereochemistry. Chemistry of titanium, vanadium, chromium, manganese sub-group elements, iron, cobalt, nickel, platinum metals, copper and zinc sub-group elements, group III, IV, V, VI, VII and rare gases with reference to isolation, properties, uses and important compounds.

Texts/References

F. A. Cotton and G. Wilkinson, *Basic Inorganic Chemistry*, Wiley Easter, 1978.
M. J. Sienko and R .A. Plane, *Chemical Principles and Properties*, McGraw Hill, 1975.
J. D. Lee, *Concise Inorganic Chemistry*, Van Nostrand Reinhold, 1977.

CH211 Chemical thermodynamics

Thermodynamic functions, laws of thermodynamics, properties of entropy, criteria for spontaneity and equilibrium, properties of free energy, Gibbs and Maxwell's relations. Chemical potential, ideal and real gases, properties of fugacity, mixing and excess functions. Chemical equilibrium, Le Chatelier's principle, partial molar quantities, standard states. Phase equilibrium involving one, two and three components. Equilibrium in condensed phases: ideal solution and colligative properties, binary solutions and azeotropes. Non-ideal systems, activity and activity coefficients. Thermodynamic formulation of surface phenomonena.

Text/ Reference

1. P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th edition, Oxford University Press, 2006.
2. G. W. Castellan, *Physical Chemistry*, 3rd edition, Addison - Wesley/Narosa Publishing House, 1993.
3. G. N. Lewis and M. Randall, *Thermodynamics*, (Revised by K. S. Pitzer and L. Brewer), International Students Edition, McGraw Hill, 1961.

CH 215 Physical Chemistry Lab -I 0 0 4 4

Potentiometry, Electrode potentials, activity coefficient, titration/s, solubility product.Condutometry, titration/s, dissociation of weak acid as a function of concentration.Ionization constant by spectrophotometry, enzyme kinetics, use of immobilized enzyme electrode, adsorption isothem, M.O. methods in chemistry .

CH 218 Organic Chemistry Lab -I 0 0 4 4

Determination of physical constants, purifi-cation of solids and liquids and methods of checking their purity. Separation of enantiomers and measurements of optical rotation. Studies of electrophilic/nucleophilic substitution reactions, redox reactions.

CH 22A Structure and Stereochemistry

Frontier molecular orbitals and organic reactions: Introduction to HOMO and LUMO, classification of nucleophiles and electrophiles based on frontier orbitals, importance of

antibonding orbitals; a brief introduction to pericyclic reactions, orbital symmetry considerations in Diels-Alder and electrocyclic reactions. [6 hrs]

Stereochemistry: Concept of chirality, center and axis of chirality, examples of compounds with one and two chiral centers, enatiomers and diastereomers, prochiral faces, enantio and diastereotopicity, absolute and relative configuration, configuration descriptors *R*/*S* and *E*/*Z* notations, optical purity, enantio/diastereomeric excess. [12 hrs]

Introduction to spectroscopic techniques: Ultraviolet and visible spectroscopy: electronic transitions, Beers law, interpretation of UV-VIS spectra, Woodward-Fieser rules.
Infrared Spectroscopy: molecular vibrations and Hooke's law, IR active and IR inactive vibrations, characteristic IR absorptions of important functional groups.
Mass spectrometry: different methods of ionization (EI, CI, electrospray, laser desorption),
molecular ion and fragment peaks, common fragmentation pathways
Nuclear Magnetic Resonance (NMR) spectroscopy: brief introduction to theory behind NMR, magnetic shielding by electrons, measurement of ^{1}H and ^{13}C chemical shifts, characteristic values of chemical shifts for various functional groups,theory of spin-spin coupling, C^{13} spectra and proton-decoupling
Basic applications of these spectroscopic methods to problem solving. [12 hrs]

Reactions of aromatic compounds: Energy profile diagrams of electrophilic aromatic substitution reactions; Nucleophilic aromatic substitutions: addition-elimination mechanism, elimination-addition mechanism (benzynes) [5 hrs]

Tutorials [10 hrs]

Text/ References

1) K. P. C. Volhardt and N. E. Schore "*Organic Chemistry: Structure and Function*", 5th Ed., W. H. Freeman and Company, **2007**.
2) L. G. Wade Jr. "*Organic Chemistry*". 7th Ed., Prentice Hall, **2009**
3) T. W. G. Solomons, C.G. Fryhle. "*Organic Chemistry*", 9th Ed., Wiley-India, **2008**.
4) J. Clayden, N. Greeves, S. Warren and P. Wothers, "*Organic Chemistry*", 1st Ed., Oxford University Press, **2001**.
5) F. A. Carey and R. J. Sundburg, "*Advanced Organic Chemistry, Part A&B*", 5th Ed., Plenum Press, **2007**.

CH 222 Reactions of carbonyl compounds

Nucleophilic Addition to CO group: MO aspects, Hydration and cyanohydrin reaction, thermodynamic Vs. Kinetic control, Organometallic reagents for C-C bond formation (organo lithium, magnesium and cerium compounds), ortholithiation, transmetallation, metal halogen exchange, Stereochemistry of nucleophilic addition to carbonyl group, Conjugate addition reactions.

Nucleophilic substitution at C=O: nature of leaving group, carbonyl reactivity, hydrolysis of esters, amides and nitriles, esterification, transesterification, conversion of acid into acid derivatives, making ketones and aldehydes from esters.

Nucleophilic substitution at C=O with the loss of carbonyl oxygen: acetals, cyclic acetals, thioketal, imines, enamines, reductive amination, alternative methods for amines formation, LAH reduction of amides, Strecker synthesis of amino acids, Wittig reaction

Enols, enolates and reactions: Alkylation, kinetic and thermodynamic enolates, Aldol reaction, specific enol equivalents (lithium enolate, aza enolate, silyl enol ether, enamines, zinc enolates), Knoevenagel reaction, Perkin reaction, Reformatsky reactions, Cannizaro reaction, Mannich reaction, intramolecular aldol reaction, Acylation, Claisen condensation, Dieckman cyclization, Conjugate addition of enolates, Robinsons Annulation

Chemoselectivity: chemoselective oxidation of alcohols to carbonyl compounds, chemoselective reduction of carbonyl compounds.

Retrosynthesis : Introduction to retrosynthetic analysis

Texts/ References

6) J. Clayden, N. Greeves, S. Warren and P. Wothers, "Organic Chemistry", First Ed., Oxford University Press, **2001**.
7) K. P. C. Volhardt and N. E. Schore "*Organic Chemistry: Structure and Function*", 5th Ed., W. H. Freeman and Company, **2007**.
8) L. G. Wade Jr. "*Organic Chemistry*". 7th Ed., Prentice Hall, **2009**.
9) T. W. G. Solomons, C.G. Fryhle. "*Organic Chemistry*", 9th Ed., Wiley-India, **2008**.
10) F. A. Carey and R. J. Sundburg, "*Advanced Organic Chemistry, Part A&B*", 5th Ed., Plenum Press, **2007**.

CH 2BC Co-ordination Chemistry

Valence bond theory, crystal field theory, molecular orbital theory and their applications, inner sphere electron transfer, outer sphere electron transfer, classification of ligands, trans effect, stability constant, Jahn-Teller effect, ploynuclear complexes, reaction of coordination compounds.

Texts/References

Peter Atkins, Peter William Atkins, Duward F. Shriver, Inorganic Chemistry, Oxford University Press, 5th edition, 2010.

Norman Greenwood and A. Earnshaw, Chemistry of the Elements, Elsevier, 2nd edition, 1997.

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

Catherine E. Housecroft, A. G. Sharpe, Inorganic chemistry, Prentice Hall, 2nd edition, 2005.

CH 423 Organic reactions

Classification of reactions: A brief introduction to substitution, elimination, addition, oxidation, reduction, rearrangement and pericyclic reactions.
Functional group transformations: alcohols to alkylating agents, Mitsunobu and related reactions, introduction of functional groups by nucleophilic substitution at saturated carbon, nucleophilic cleavage of C-O bonds in ethers and esters and inter-conversion of carboxylic acid derivatives
Oxidation: Metal based oxidizing reagents: A review and detailed discussion of chromium, manganese, ruthenium, silver and other metal based reagents. Non-metal based oxidizing reagents: DMSO, peroxide, peracid and oxygen based oxidation. Miscellaneous oxidizing reagents like IBX, DMP, CAN, DDQ, periodate etc.
Reduction: Homogeneous and heterogeneous; Discussion on borane based racemic and chiral reagents, hydrogenations aluminium, tin, silicon based reducing agents. Dissolving metal reductions.
Selectivity and protecting groups: Illustration of chemoselectivity, regioselectivity and stereoselectivity with examples; protecting groups for alcohols, amines, acids, ketones and aldehydes.
Cycloaddition reactions: Diels-Alder reaction; general features, dienes, dienophiles, selectivity, intramolecular and intermolecular reactions, hetero-Diels Alder reaction. 1,3-dipolar cycloaddition reactions; general features, dipoles, dipolarophiles. [2+2] cycloaddition reactions; general features, selected examples.
Molecular rearrangements: Illustration of electron deficient and electron rich skeletal rearrangements with examples; Sigmatropic rearrangements-Claisen and related rearrangments, Cope and oxy-Cope rearrangements; 2,3-sigmatropic rearrangements and ene reaction.

Text/ References

11) Jerry March, "*Advanced Organic Chemistry*", Fifth Ed., Wiley, **2007**.

12) F. A. Carey and R. J. Sundburg, "*Advanced Organic Chemistry, Part B*", Fifth Ed., Plenum Press, **2007**.
13) J. Clayden, N. Greeves, S. Warren and P. Wothers, "Organic Chemistry", First Ed., Oxford University Press, **2001**.
14) W. Carruthers, "*Some Methods of Organic Synthesis*", Cambridge University Press,
15) K. Peter C. Vollhardt and Neil E. Schore "Organic Chemistry" W. H. Freeman and Company, **1999**.

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 ABC Electrochemistry of Solutions and Interfaces

Brief review of chemical thermodynamics. Electrochemistry of solutions : Ion-solvent interactions, ion-ion interactions, ionic migration and diffusion. Thermodynamics of galvanic cells: Equilibrium electrode potentials, IUPAC convention for electrode potentials, classification of electrodes. Origin of emf and classification of electrochemical cells. Redox equilibria in bioenergetics and metabolism. Electron transfer at the electrode-solution interface, Voltammetry, fuel cells, corrosion.

Text / References

L. I. Antrapov, Theoretical Electrochemistry, Mir Publishers, 1972.
J. J. O'M. Bockris and A. K. N. Reddy, Modern Electrochemistry, Vol. 1 and 2, 2nd edition, Plenum Press, 1998.
P. Atkins and J. de Paula, Atkins' Physical Chemistry, 8th edition, Oxford University Press, 2006.
Fundamentals of Electrochemistry, 2nd ed, Bagotsky, V.S., Hoboken: Wiley-Interscience 2006.

CH 437 Advanced transition metal chemistry 2 1 0 6

General chemistry of the d-block and f-block elements, structure-reactivity correlation, magnetic properties, electron- transfer aspects, spectroscopic features, reaction kinetics, transition metal ions in biological processes, supramolecular chemistry.

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.

Russell S. Drago, Physical Methods in Inorganic Chemistry, Cengage Learning, 1992.

Catherine E. Housecroft, A. G. Sharpe, Inorganic chemistry, Prentice Hall, 2nd edition, 2005.
Jean-Marie Lehn, Supramolecular Chemistry: Concepts and Perspectives, VCH, 1995

CH 4AB Inorganic Chemistry Lab -II 0 0 4 4

Complex material analyses: minerals/ alloys. Quantitative estimations using conductometry and spectrophotometry. Estimation of iron in iron ore. Estimation of mixture of metal ions by EDTA titrations. Karl-Fischer Titration.

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 4KP Organic Chemistry Lab -II **0 0 4 4**

Qualitative analysis of organic compounds. Chemical separation of binary mixtures and their qualitative analysis.

Texts/References

R. L. Shriner, R. C. Fuson and D.Y. Curtin, *Systematic Identification of Organic Compounds, a lab. manual*, 6th edition Wiley, New York

CH 416 Physical Organic Chemistry **2 1 0 3**
(Half Semester)

Symmetry-adapted orbitals. Mixing rules and buildup approach to molecules and molecular complexes. Energy surface for bond breaking and making. Kinetic vs thermodynamic control, Curtin-Hammett principle, Hammond Postulate Reactive intermediates: Carbocations, carbanions, carbenes, benzyne. Empirical scales for electronic, steric, and solvent effects. Mechanism according to free-energy correlation and correpondence with theory of orbital interaction. Illustrative examples. Linear free energy relationship, Hammett and Taft equations

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 4GP Thermal and photochemical reactions **2 1 0 3**
(Half semester)

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. 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 pericyclic reactions. Cycloaddition reactions. FMO, orbital and state correlation diagrams, and aromatic transition state approaches. Various [2+2] and [4+2] cycloaddition reactions. Alder 'Ene Reaction'. Sigmatropic reactions. Photochemical cycloadditions. Cheletropic reactions.

Text/References

1. R. B. Woodward and R. Hoffmann, *"The Conservation of Orbital Symmetry"*, Academic Press, New York, 1971.
2. M. J. S. Dewar and R. C. Dougherty, "*The PMO Theory of Organic Chemistry*", Plenum Press, New York, 1975.
3. T. L. Gilchrist and R. C. Storr, "*Organic Reactions and Orbital Symmetry"*, 2nd Edn., Cambridge University Press, Cambridge, 1979.
4. R. P. Wayne, *"Principles and Applications of Photochemistry"*, Oxford Science Publications, Oxford University Press, Oxford, 1988.
5. A. Gilbert and J. Baggot, "*Essentials of Molecular Photochemistry*", Blackwell Scientific Publications, Oxford & Boston, 1991.
6. M. Klessinger and J. Michl, "*Excited States and Photochemistry of Organic Molecules*", VCH Publishers, Inc., New York, 1994.
7. I. Fleming, "*Pericyclic Reactions*", Oxford University Press, Oxford, 1998.
8. A. Rauk, "*Orbital Interaction Theory of Organic Chemistry"*, 2nd Edn., Wiley Interscience, New York, 2001.
9. S. Sankararaman, "*Pericyclic Reactions- A Textbook*", Wiley-VCH, Weinheim, 2005.

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 442 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 4XY Molecular Energetics and Dynamics

Statistical view of entropy. Laws of thermodynamics from statistical considerations Molecular view of temperature and heat capacity. Boltzmann distribution. Thermodynamic quantities in terms of partition functions. Statistical mechanics of simple gases and solids. Equilibrium constant in terms of partition functions. Bose-Einstein and Fermi-Dirac statistics. Overview of rate laws and determining rates and orders of reactions. Complex Reactions. Catalysis. Temperature dependence and Arrhenius law. Potential energy surfaces. Kinetic theory of collisions. Transition state theory. RRK and RRKM theories. Reaction cross-sections, rate coefficients, reaction probabilities. Photochemical reactions. Ultrafast reactions. Diffusion in solids, liquids and solutions. Chemical oscillations and nonlinear dynamics.

Text/ References

Molecular Driving Forces: Statistical Thermodynamics in Chemistry and Biology/ by K. A. Dill and S. Bromberg, Garland Science, 2003.

Molecular Thermodynamics by D. A. McQuarrie, and J. D. Simon, Viva Books, 2004.

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

Chemical Kinetics by K. J. Laidler, 3rd Edition, Prentice Hall, 1987.

Chemical Kinetics and Dynamics by J. I. Steinfeld, J. S. Francisco and W.L. Hase, 2nd Edition, Prentice Hall, 1999.

Chemical Kinetics and Reaction Dynamics by P. L. Houston McGraw-Hill Higher Education, 2001.

CH 4CP Bioinorganic chemistry

Introductory awareness of the role of metal ions in biology and medicine. A quick refresh of the general features of coordination chemistry, bio-molecules, spectral and biochemical techniques.

Bioinorganic approach with respect to the following aspects: Transport of alkali and alkaline earth ions and functioning of ATPases. Vanadium in haloperoxidases and nitrogenases. Role of manganese in the oxygen evolution cluster of photosystem – II. Iron proteins & Enzymes: Transport & storage; Porphyrin and non-porphyrin based: Electron Transport; Monooxygenases, Dioxygenases; Phosphatases; Reductases; Superoxide dismutase. Cobalt: Cobalamine based enzymes. Nickel: Urease; Hydrogenases; Carbonmonooxide Dehydrogenases. Copper: Electron Transport; Oxidases; Monooxygenases; Dioxygenases; Various types of copper centers; Super oxide dismutase. Zinc: Hydrolases; Peptidases; Lyases; Ligages; Oxido-reductases; Transferases. Molybdenum: Nitrogenase; all types of Oxido-reductases. Selenoenzymes; Nitrosyls in bioinorganic chemistry.

Text

1. Bioinorganic Chemistry: The Biological Chemistry of Transition Metals, Michael Watkinson, 2009, John Wiley & Sons
2. Principles of Bioinorganic Chemistry, Stephen J. Lippard, Jeremy Mark Berg, 1994, University Science Publications
3. Inorganic Biochemistry: An Introduction, James A Cowan, 1993, VCH Publishing.

References

4. Handbook on metalloproteins, Ivano Bertini, Astrid Sigel, Helmut Sigel, 2001, CRC Press
5. Bioinorganic chemistry: transition metals in biology and their coordination chemistry, Alfred Trautwein, 1997, Deutsche Forschungsgemeinschaft.
6. Bioinorganic Chemistry- an inorganic perspective of life, D. P. Kessissoglou, 1995, Kluwer Academic.

CH 481: Chemistry and Computers **2 0 2 6**

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 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 prepara- tions involving different techniques. Isolation of natural products.

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 sepectroscopy. 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 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 H_2 evolution, photoelectrochemical solar cells.

Vacuum measurement. IR spectrum of HCl, Use of M.O. theory, solution of Schrodinger equation for polyatomics.

CH 507 Methods in organic synthesis

Reaction vs synthetic method; metal atom functionality in organometallic reactions, organometallics as protecting and stabilizing groups, palladium catalyzed reactions, Heck reaction, cross coupling reactions (Suzuki, Stille, Negishi, Kumada, Hiyama, Sonogashira, Buchwald-Hartwig), Fischer carbenes, Schrock carbenes, Olefin metathesis, various types of metathesis and application to organic synthesis, Dotz benzoannulation, Pauson-Khand reaction, [2+2+2] cycloadditions, Grignard reactions, Rieke magnesium, 1,2 vs 1, 4-addition, cerium reagents, copper reagents, homocuprates, lower order cuprates, higher order cuprates, chromium arene complexes and reactions, McMurry coupling, role of silicon in organic synthesis, origin and consequence of alpha effect and beta effect involving silicon compounds, role of silicon in few name reactions. Some selected natural and non-natural product synthesis involving these reactions.
Concise introduction to asymmetric synthesis, detailed discussion on resolution, chiral auxiliaries, chiral ligands, chiral catalysts and organocatalysts with specific examples.
Introduction to domino/tandem/cascade reaction concepts with selected examples

Text/ References

G. S. Zweifel and M. H. Nantz, Modern Organic Synthesis-An Introduction, W. H. Freeman and Company, 2006
B. M. Trost and I Fleming, Comprehensive organic synthesis, Pergamon Press, 1992.
Organanometallics in Organic Synthesis, J. M. Swan, D. St. C. Black, Chapman and Hall, London, 1974
Organotransition Metal Chemistry: Applications to Organic Synthesis, S. G. Davis, Pergamon Press, Oxford, 1982.
Basic Organometallic Chemistry, B. D. Gupta, A J Elias, Universities Press, Chennai, 2010
Transition Metals in the total synthesis of complex organic molecules, L. S. Hegedus, University Science Books, 1994.

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 ^{1}H,^{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. Morril, *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 546 Bioorganic chemistry

Aminoacids, peptides and proteins: Amino acids: structure, acid-base chemistry, and chemical synthesis; peptide bond formation and coupling reagents-carbodiimides and phosphonium reagents; orthogonal protecting groups; solid-phase peptide synthesis: (Fmoc/Boc strategies); native peptide ligation; cyclic peptides; amino acid analysis and peptide sequencing; brief introduction to ribosomal protein synthesis; combinatorial chemistry; enzyme chemistry: proteases and phosphotases; proteins as drug targets.

Carbohydrates: Introduction to carbohydrates; structure, configuration and conformation; common protecting groups and protecting group strategies; glycosylation: general concepts, various methods of glycoside bond formation; strategies in oligosaccharide synthesis: automated and enzymatic approaches; glycoconjugates: glycolipids and glycoproteins; fundamentals of glycobiology; tools for glycomics; carbohydrate based drug discovery.

Nucleosides, nucleotides and nucleic acids: Introduction to nucleic acids: biological importance, discovery, structure; chemical synthesis of nucleosides and protecting groups for nucleobase, sugar and phosophates; solution and solid phase synthesis of oligonucleotides: phosphotriester, H-phosphonate and phosphoramidite strategies; DNA Processing Enzymes: DNA polymerases, ligases, restriction endonucleases, PCR; enzymatic synthesis of nucleic acids; principle behind sequencing; nucleic acid as drug targets; quadruplex nucleic acids; nucleic acids based enzymes: ribozymes, DNA enzymes and riboswitches; nucleic acid based therapeutic strategies: antisense, RNA interference and aptamers; DNA damage and repair.

Student Presentations

Text/ References

1) P. Lloyd-Williams, F. Albericio, E. Giralt, *Chemical Approaches to the Synthesis of Peptides and Proteins*, 1st Edition, CRC Press, Boca Raton,**1997**
2) S. Doonan, *Peptides and Proteins*, 1st Edition, RSC Publishing House, London, **2002**
3) T. Bugg, *An Introduction to Enzyme and Coenzyme Chemistry*, 2nd Edition, Blackwell Science, Oxford, **2004**
4) B. G. Davis & A.J. Farbanks, *Carbohydrate Chemistry*, 1st Edition, Oxford University Press, **2002**
5) R. V. Stick., *Carbohydrates: The Essential Molecules of Life*, 2nd Edition, Academic Press, **2009**
6) D. E. Levy and P. Fugedi, *The Organic Chemistry of Sugars*, CRC Press, **2006**
7) G. M. Blackburn, M. J. Gait, D. Loakes, D. M. Williams, *Nucleic Acids in Chemistry and Biology*, 3rd Edition, RSC Publishing, London, **2006**
8) S. Doonan, *Nucleic Acids*, 1st Edition, RSC Publishing House, London, **2004**
9) A. Lehninger, D. L. Nelson, Cox, M. M. *Principles of Biochemistry*, 5th Edition, W.H Freeman, **2008**

CH 547 Organometallic chemistry and catalysis

Introduction; factors guiding metal-carbon bond formation; general synthetic methods for Main Group organometallics, structure and bonding of alkali, alkaline-earth organometallics, EAN rule, classification of carbon-based ligands by donor atoms and no of electrons donated by the ligand, sigma-donor and pi-acceptor-; transition metal organometallics; reactivity studies, applications of organometallic compounds in homogenous catalysis; hydrogenation, carbonylation, metal-mediated C-X (X = C, heteroatom) bond formations, olefin metathesis and Zieglar-Natta polymerization, stereochemistry, applications in asymmetric synthesis.

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 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 510 Heterocyclic chemistry

1. Introduction to heterocyclics and their importance.
2. Nomenclature of ring systems
   (a) Trivial System (b) Replacement system (c) Fusion system
   (d) Hantzsch-Widman nomenclature
3. Structure, reactivity and synthesis of reduced three membered Heterocycles
   (a) Oxirane: Sharpless method, Shi epoxidation, Jacobsen epoxidation, etc
   (b) Thiirane (c) Aziridine
4. Structure, reactivity and synthesis of reduced four membered Heterocycles
   (a) Oxetane (b) Thietane (c) Azetine
5. Structure, reactivity and synthesis of reduced five membered Heterocycles
   (a) Pyrrole: Paal Knorr, Hantzsch Methods, etc
   (b) Thiophene: Paal Knorr, Hinsberg method, etc
   (c) Furan: Paal Knorr, Fiest-Benary, Industrial Method, etc
   (d) Pyrazole, Imidazole, Oxazole, Thiazole
   (e) Synthesis using modern methods
6. Structure, reactivity and synthesis of reduced Six membered Heterocycles
   (a) Pyridine: Synthesis, heterynes, pyridones, N-oxides
7. Aromatic heterocyclics
   a) Indole: Fischer indole synthesis, Bischler synthesis, Madelung synthesis, Domino and cascade methods of indole synthesis
   b) Quinoline and Isoquinoline
   c) Coumarins and Chromones
8. Polyhetero ring systems: Click chemistry in heterocycle synthesis
9. Synthesis of selected heterocylic natural products
10. Some modern methods of heterocycle synthesis with emphasis on organometallic reagents

Text/ References

1] Topics in Heterocycles Chemistry. G. W. Gribble. Spinger-Verlag Berlin Heidelberg, 2010.
2] Modern Heterocyclic Chemistry. 4 Volume Set. Julio Alvarez-Builla, Juan Jose Vaquero, José Barluenga. Wiley. 2011.
3] L.A. Paquette, Principles of Modern Heterocyclic Chemistry, W.B.
Benjamin, Inc., 1978.
4] Handbook of Heterocyclic Chemistry. Alan R. Katritzky and A. F. Pozharskii, Elservier 2000.
6] The Chemistry of Heterocycles. T. Eicher, S. Hauptmann, Wiley-VCH 2003
5] R. K. Bansal, Heterocyclic Chemistry, Synthesis, Reactions and
Mechanisms, Wiley Eastern Ltd., 1990.
6] J.A.J. Joule and G.F. Smith, Heterocyclic Chemistry, ELBS, 2nd Ed., 1982.
7] F.G. Riddell, The Conformational Analysis of Heterocyclic Compounds,
Academic Press, 1980.
8] B.M. Acheson, An Introduction to the Chemistry of Heterocyclic
Compounds, Interscience, 2nd Ed., 1975.

CH XXX Advanced Coordination Chemistry

Origin of supramolecular chemistry, fundamental supramolecular interactions (covalent bonds, ionic interactions, ion-dipole interactions, dipole-dipole interactions, hydrogen bonds, cation-π interactions, π-π interactions, vander Waals forces, hydrophobic effects). Supramolecular design, host-guest chemistry, molecular self-assembly, supramolecular applications in biomedical sciences, supra molecular catalysis, supramolecules as nanoscale devices.
Introduction to magneto-chemistry of coordination compounds, origin of magnetism, classes of magnetism, spin and orbital contribution to magnetic moments, measurement of magnetic susceptibility using common experimental protocols, temperature dependency of magnetic susceptibility, single-ion magnetic properties, Van Vleck equation and its applications, magnetic anisotropy and zero field splitting in coordination compounds, spin-crossover in coordination complexes, mechanism of spin crossover and LIEEST. Superexchange interaction in homo and hetero dinuclear and oligonuclear complexes, Bleany-Bowers equation, orbital interaction in molecular magnetism, Magneto-structural correlations in dinuclear complexes. Single Molecule Magnets and its related phenomena in molecular clusters.

Texts/References

1. J. W. Steed, J. L. Atwood, *Supramolecular Chemistry*, 2nd edition, Wiley-VCH Inc.,2009.

2. P. J. Cragg, *Supramolecular Chemistry: from biological inspiration to biomedical applications*, Springer Science, 2010.
3. O. Kahn, *Molecular Magnetism*, Wiley-VCH Inc., 1993.
4. D. Gatteschi, R. Sessoli, J. Villain, *Molecular Nano Magnets*, Oxford University press, 2006.
5. R. S. Drago, *Physical Methods for Chemists*, Saunders, 1992.

CH 540 Introduction to Medicinal Chemistry

Drug discovery an overview, production of drugs, classification of drugs, drug nomenclature, how drugs work, methods of drug development, patterns of healthcare, overview of pharmaceutical industry, drug targets, drug metabolism, pro drugs, pharmacokinetics and related topics, enzyme inhibition and inactivation, enzymes as drug targets, receptors as drug targets, production of drugs, chirality and biological activity, selected examples of drug mechanisms, selected examples of the following drugs: NSAID, steroids, antibacterials, anticancer, antiulcer, drugs related to tropical diseases, antivirals, antihistamines

References:

The Organic Chemistry of Drug Design and Drug Action, R. B. Silverman, Academic Press, London, 1992.
An Introduction to Medicinal Chemistry, G. L. Patrick, Oxford, London, 2009.
Pharmaceutical Chemicals in Perspective, B. G, Reuben, H. A. Wittcoff, John Wiley, New York, 1989.
Core Concepts in Pharmacology, L. N. Holland, Jr., M. P. Adams, Pearson, New Jersey, 2007.
Drug-like properties: Concepts, structure design and methods, E. H. Kerns, L Di, Academic Press, New York, 2008,
Molecules and Medicine, E. J. Corey, B. Czako, L. Kurti, John Wiley, New Jersey,2007.
Molecules that changed the world, K. C. Nicolaou, T. Montagnon, Wiley-VCH, Weinheim, 2008.

CH 556 Polymer Chemistry

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

George Odian, Principle of Polymerization (3rd Edition), New York, John Wiley, 1991
P. J. Flory, Principles of Polymer Chemisty, Cornell University Press, 1953
Manas Chanda, Advanced polymer chemistry:a problem solving guide, New York: Marcel Dekker, 2000
Fred W. Billmeyer Jr., Textbook of Polymer Science (3rd Edition), John Wiley, 1991

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

General comparision 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 5ZX; Macromolecular Crystallography

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, sulpur 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 528 Natural Products **2 1 0 6**

Terpenoids : Classification, structure, chemistry and biogenesis of some important mono; sesqui,di, and triter penes.
Steroids : Sterols and bile acids, estrogens, androgens, gestogens 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, xanthones, quinones, pterins, chlorophyll and haemin.
Carbohydrates: Stereochemistry, reaction and conformation of monosaccharides, deoxy and aminosugars, hexonic acid and vitamin C, disaccharides, polysaccharides, inositol; gan- gliosides 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 Carbohydratres*, 3rd edition, Clarendon Press, 1968.
T. A. Geissman, *Chemistry of Flavonoid Compounds*, Pergamomn Press, 1962.

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, general ized 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. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, *Vol.1 and 2*, Plenum Press, 1998.
Industrial Electrochemistry, 2nd ed, Pletcher, Derek/Walsh, Frank C.,
London: Chapman and Hall, 1990
Electrochemistry for Chemists, 2nd ed, Sawyer, Donald T./Sobkowiak,
Andrej/Roberts, Julian L., New York: John Wiley, 1995
Transient Techniques in Electrochemistry, Macdonald, Digby D., New York:
Plenum Press, 1977

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, nonstoichimetry 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 Dyamics 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. Photoelectochemistry of excicted 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 588 Organic Synthesis 2 1 0 6

Strategy and design of organic synthesis: Introduction, scope and a brief history of organic synthesis, synthetic strategy, retro-synthesis, analysis and practice of total synthesis, linear and convergent synthesis.
Concepts of synthetic equivalents and Umpolung: benzoyl and acyl anion equivalents, dithianes, enol ethers and nitro compounds.
Carbon-Carbon bond formation: alkylation of enolates, enamines and hydrazones, alkylation of heteroatom stabilized anions, organometallic reagents.
Carbon-Carbon double bond formation: aldol condensation, Wittig and related reactions, Peterson olefination, Julia-Lythgoe olefination, carbonyl coupling reaction (McMurry reaction), Tebbe reagent, Shapiro and related reactions, β-elimination and dehydration, From diols and epoxides, from acetylenes, from other alkenes (olefin metathesis and transition metal catalyzed cross coupling reactions).

Carbon-Carbon triple bond formation: from other acetylenes, from carbonyls, from olefins, from strained rings, Eschenmosher fragmentation, allenes etc.

3-Membered rings: **Epoxides**- using peracids, hydroperoxides and dioxiranes; transition metal catalyzed epoxidation, halohydrins, Darzen's condensation, sulfur ylides. **Cyclopropanes**-Simmons Smith reaction, diazo compounds, sulfur ylides and SN2 displacements. **Aziridines**-nitrenes and SN2 displacements.

4-Membered rings: Various methods of forming cyclobutanes, cyclobutenes and oxetanes

5-Membered rings: intramolecular SN2 reactions, intramolecular Michael and aldol condensation reactions, intramolecular Wittig olefination, ring expansion and contraction reactions, 1,3-dipolar cycloaddition reactions, Nazarov cyclization, arene-olefin photocycloaddition, radical cyclization reactions.

6-Membered rings: Diels-Alder reaction, o-quinodimethanes, cation olefin cyclization, Robinson annulations

Biosynthesis: biogenesis and biosynthesis; biosynthetic pathways of some mono, sesqui and diterepenes and steroids.

Selected synthesis of natural products: Total synthesis of several triquinanes, platensimycin, perhydrohistrionicotoxin, progesterone, estrone, prostaglandins, cubane, taxol and epothilones.

Suggested books

1. David J. Hart "Organic *Synthesis via Examination of Selected Natural Products*" World Scientific, **2011**
2. S. Warren, "*Designing Organic Syntheses"*, John Wiley & Sons **2009.**
3. G. S. Zweifel and M. H. Nantz. "Mdern Organic Synthesis-An Introduction",W. H. Freeman and Company, **2006**.
4. R. O. C. Norman and J. M. Coxon "*Principles of Organic Synthesis*" Nelson Thornes, Third Edition, **2005**.
5. Michael B. Smith and Jerry March, "*March's Advanced Organic Chemistry*", Fifth Ed., Wiley, **2001**.
6. K. C. Nicolaou, E. J. Sorenson, "*Classics in Total Synthesis, I, II and III"*
7. B. M. Trost and I. Fleming, "*Comprehensive Organic Synthesis*", Pergamon Press, **1992**.
8. T.W. Greene, "*Protecting Groups in Organic Synthesis"* (3rd edition), J. Wiley & Sons, **1999**.
9. F. A. Carey, R. Sundberg, , "*Advanced Organic Chemistry, Part B*", 2nd Ed., Plenum Press, **1990**.
10. E. J. Corey, X. Cheng, "*The Logic of Chemical Synthesis"*, John Wiley **1989**.
11. W. Carruthers, "*Some Modern Methods in Organic Synthesis"*, Cambridge University Press **1989**.
12. S. Warren, "*Organic Synthesis: The Disconnection Approach"*, John Wiley & Sons.

CH XXX: X-ray Crystallography

Geometric Crystallography: Lattices, point groups and space groups, and lattice transformations. Processing raw diffraction data: Diffraction data statistics, temperature & scale factor determination, density measurements and calculations, molecular formula and molecular weight determination, space group determination. (c) Structure determination: Heavy atom Patterson methods, direct methods, isomorphous replacement methods. Refinement: isotropic and anisotropic, atom fix and hydrogen fixations, riding models. Interpretation of the structural data: metric parameters, dihedral data, H-bond data, preparation of structure plots including ORTEP and lattice structures including packing diagrams. Practical exercise of structure determination using standard packages: one centro-symmetric and one non-centrosymmetric crystal data.

Texts/References

X-ray structure determination: A practical guide, G.H. Stout and L.H. Jensen, Wiley, Second Edition 1989.

Foundations of Crystallography with Computer Applications, M.M. Julian, CRC Press, 2008.

An Introduction to X-ray Crystallography, M.M. Woolfson, Cambridge University Press; 1970.