Integrated M.Sc. and 2 year M. Sc. Curricula

Department of Chemistry
Indian Institute of Technology Bombay

CURRICULUM FOR 5 YEAR INTEGRATED M.Sc. PROGRAMME

First year : First Semester

Code	Name	L	T	P	C
CH 103	Chemistry-I	2.0	1.0	0.0	6.0
CS 101	Computer programming and utilization	2.0	1.0	0.0	6.0
MA 105	Calculus	3.0	1.0	0.0	8.0
HS 101	Economics	2.0	1.0	0.0	6.0
CH 117	Chemistry Lab	0.0	0.0	3.0	3.0
ME 113	Workshop practice	0.5	0.0	3.0	4.0
		9.5	4.0	6.0	33.0

Contact hours: 19.5
Credits: 33.0

First year : Second Semester

Code	Name	L	T	P	C
CH 104	Chemistry-II (DIC)	2.0	1.0	0.0	6.0
PH 105	Physics-II (Modern Physics)	2.0	1.0	0.0	6.0
MA 106 MA 108	Linear algebra (half semester) Ordinary differential equations (half semester)	3.0	1.0	0.0	8.0
IC 102	Data analysis and interpretation	2.0	1.0	0.0	6.0
PH 117	Physics Lab	0.0	0.0	3.0	3.0
ME 118	Engineering graphics and drawing	1.0	0.0	3.0	5.0
		10.0	4.0	6.0	34.0

Contact hours: 20.0
Credits: 34.0

Second year : First Semester

Code	Name	L	T	P	C
CH 211	Physical Chemistry - I	2.0	1.0	0.0	6.0
CH 221	Organic Chemistry - I	2.0	1.0	0.0	6.0
BT 251	Molecular Cell Biology	2.0	1.0	0.0	6.0
EE 101	Introduction to electrical and electronic circuits	3.0	1.0	0.0	8.0
CH 206	Inorganic Chemistry Lab -I	1.0	0.0	3.0	4.0
IC 211	Experimentation and measurements lab	0.0	0.5	3.0	4.0
		10.0	4.5	6.0	34.0

Contact hours: 20.5
Credits: 34.0

Second year : Second Semester

Code	Name	L	T	P	C
CH 222	Organic Chemistry - II	2.0	1.0	0.0	6.0
CH 210	Inorganic Chemistry - I	2.0	1.0	0.0	6.0
CL 152	Elements of Chemical Engineering	2.0	1.0	0.0	6.0
PH 103	Electricity and Magnetism	2.0	1.0	0.0	6.0
ES 200/	Environmental science and engineering/	3.0	0.0	0.0	3.0
HS200	Environmental studies (Half-semester courses)	3.0	0.0	0.0	3.0
CH 215	Physical Chemistry Lab - I	0.0	0.0	4.0	4.0
		14.0	4.0	4.0	34.0

Contact hours: 22.0
Credits: 34.0

Third year : First Semester

Code	Name	L	T	P	C
CH 423	Organic Chemistry -III	2.0	1.0	0.0	6.0
CH 427	Chemical and Statistical Thermodynamics	2.0	1.0	0.0	6.0
PH 201	Optics	2.0	1.0	0.0	6.0
IE1	Institute Elective from HSS	3.0	0.0	0.0	6.0
CH 317	Organic Chemistry Lab - I	0.0	0.0	4.0	4.0
EP 215	Electronics Lab - I	0.0	0.0	3.0	3.0
		9.0	3.0	7.0	31.0

Contact hours: 19.0
Credits: 31.0

Third year : Second Semester

Code	Name	L	T	P	C
CH 416	Physical Organic Chemistry	2.0	1.0	0.0	6.0
CH 426	Rate Processes	2.0	1.0	0.0	6.0
CH 429	Modern Methods of Analysis	2.0	1.0	0.0	6.0
IE 2	Institute Elective	3.0	0.0	0.0	6.0
CH 316	Inorganic Chemistry Lab - II	0.0	0.0	4.0	4.0
CH 318	Organic Chemistry Lab - II	0.0	0.0	4.0	4.0
		9.0	3.0	8.0	32.0

Contact hours: 20.0
Credits: 32.0

Fourth year : First Semester

Code	Name	L	T	P	C
CH 425	Chemical Bond and Molecular Geometry	2.0	1.0	0.0	6.0
CH 438	Chemistry of Main Group Elements	2.0	1.0	0.0	6.0
CH 507	Methods in Organic Synthesis	2.0	1.0	0.0	6.0
IE 3	Institute Elective	2.0	1.0	0.0	6.0
CH 433	Physical Chemistry Lab - II	0.0	0.0	4.0	4.0
CH 419	Separation Techniques Lab	0.0	0.0	4.0	4.0
		8.0	4.0	8.0	32.0

Contact hours: 20.0
Credits: 32.0

Fourth year : Second Semester

Code	Name	L	T	P	C
CH 402	Thermal and Photochemical Reactions	2.0	1.0	0.0	6.0
CH 437	Chemistry of Transition Elements	2.0	1.0	0.0	6.0
CH 442	Molecular Spectroscopy	2.0	1.0	0.0	6.0
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
CH 418	Organic Chemistry Lab - III	0.0	0.0	4.0	4.0
		6.0	3.0	12.0	30.0

Contact hours: 21.0
Credits: 30.0

Fifth year : First Semester

Code	Name	L	T	P	C
CH 557	Topics in Chemistry	2.0	1.0	0.0	6.0
CH 547	Organometallic Chemistry	2.0	1.0	0.0	6.0
IE 4	Institute Elective	2.0	1.0	0.0	6.0
CH 521	Interpretative Molecular Spectroscopy	2.0	0.0	0.0	4.0
CH 595	Project	0.0	1.0	10.0	12.0
		8.0	4.0	10.0	34.0

Contact hours: 22.0
Credits: 34.0

Fifth year : Second Semester

Code	Name	L	T	P	C
CH EL1	Elective-I	2.0	1.0	0.0	6.0
CH EL2	Elective-II	2.0	1.0	0.0	6.0
CH EL3	Elective-III	2.0	1.0	0.0	6.0
CH EL4	Project				18.0
		6.0	3.0	0.0	36.0

Contact hours: 9.0
Credits: 36.0

Departmental electives I to III

Physical Chemistry

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

Organic Chemistry

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

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

CH 8XX courses qualify as Department Electives. Students may study them, subject to fulfillment of prerequisites, in any.

Courses from other departments can NOT be studied in lieu of department electives.

CURRICULUM FOR 2 YEAR M.Sc. PROGRAMME

First year : First Semester

Code	Name	L	T	P	C
CH 423	Organic Chemistry -III	2.0	1.0	0.0	6.0
CH 425	Chemical Bond and Molecular Geometry	2.0	1.0	0.0	6.0
CH 427	Chemical and Statistical Thermodynamics	2.0	1.0	0.0	6.0
CH 438	Chemistry of Main Group Elements	2.0	1.0	0.0	6.0
CH 433	Physical Chemistry Lab - II	0.0	0.0	4.0	4.0
CH 419	Separation Techniques Lab	0.0	0.0	4.0	4.0
CH 481	Computers in Chemistry	1.0	0.0	2.0	4.0
		9.0	4.0	10.0	36.0

Contact hours: 23.0
Credits: 36.0

First year : Second Semester

Code	Name	L	T	P	C
CH 402	Thermal and Photochemical reactions	2.0	1.0	0.0	6.0
CH 416	Physical Organic Chemistry	2.0	1.0	0.0	6.0
CH 426	Rate Processes	2.0	1.0	0.0	6.0
CH 429	Modern Methods of Analysis	2.0	1.0	0.0	6.0
CH 437	Chemistry of Transition Elements	2.0	1.0	0.0	6.0
CH 442	Molecular Spectroscopy	2.0	1.0	0.0	6.0
CH 432	Inorganic Chemistry Lab - III	0.0	0.0	4.0	4.0
CH 418	Organic 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
		12.0	6.0	12.0	48.0

Contact hours: 30.0
Credits: 48.0

Second year : First Semester

Code	Name	L	T	P	C
CH 507	Methods in Organic Synthesis	2.0	1.0	0.0	6.0
CH 521	Interpretative Molecular Spectroscopy	2.0	1.0	0.0	6.0
CH 547	Organometallic 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 595	Project				12.0
		9.0	3.0	0.0	36.0

Contact hours: 23.0
Credits: 34.0

Second year : Second Semester

Code	Name	L	T	P	C
CH EL1	Elective-I	2.0	1.0	0.0	6.0
CH EL2	Elective-II	2.0	1.0	0.0	6.0
CH EL3	Elective-III	2.0	1.0	0.0	6.0
CH 596	Project				18.0
		6.0	3.0	0.0	36.0

Contact hours: 9.0
Credits: 36.0

Electives I to III from the following :

Physical Chemistry

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

Organic Chemistry

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

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

CH 8XX courses qualify as Department Electives. Students may study them, subject to fulfillment of prerequisites, in any.

Courses from other departments can NOT be studied in lieu of department electives.

Chemistry Minor Program

Minor in Chemistry (For the BTech and DD, Total 30 Extra Credits)

1. CH 104 (Chemistry –II)
2. CH 211 (Physical Chemistry –I)
3. CH 210 (Inorganic Chemistry –I)
4. CH 221(Organic Chemistry –I)
5. CH 4XX (Any 400 level course for which prerequisites are met)
6. CH 4YZ (A second 400 level course for which prerequisites are met)

DEPARTMENTAL COURSES

PREPARATORY COURSES

CH 001 : Preparatory Chemistry I **3 2 0**

General introduction: Formula, stoichiometry, molarity, molality, normality, applications of these concepts.

Gases: Boyle's law, Charles' law, PV=nRT and applications : Dalton's law of partial pressure, Graham's law of diffusion, kinetic theory of gases (physical concept) and applications in problems solving.

Chemical Equilibrium - Ionic Equilibrium: Law of mass action, reversible reaction, equilibrium constant for homogeneous annd heterogeneous reactions, effect of pressure, volume and concentration of reactants and products on equilibrium, effect of temperature on equilibrium constant. Dissociation constants of acids and bases, common ion effect, ionisation constant of water, pH, buffer solutions and hydrolysis of salts. Solubility product and its application to chemical analysis. Determination of K_a, K_b, K_w and K_{sp} by conductance measurements. Colligative properties, fractional distillation, phase diagrams.

Thermodynamics: First law of thermodynamics, reversible work, irreversible work, isothermal and adiabatic, thermochemistry, Hess's law, bond energy. The entropy concept.

Chemical Kinetics: Rate expression, order and molecularity, first order reaction, half life period, radioactive carbondating, Arrhenius equation activation energy and catalysis.

Electrochemistry: Faraday's laws of electrolysis, galvanic cells, electrode potential and electrode reactions of simple electrode processes.

Atomic Structure and Periodic classifications: Spectra of H-atom, Bohr's model of H-atom, wave nature of electron, atomic orbitals, shapes of s,p, and d orbitals, quantum numbers, Pauli Principle, Hund's Rule, electronic configuration of elements upto Krypton, periodic classification of elements. Solids.

Texts/References

G. M. Barrow, *Physical Chemistry*, 5th edition, Tata McGraw-Hill, New Delhi, 1992

S. H. Maron and C. F.Prutton, *Principles of Physical Chemistry*, 4th Edition, Oxford & IBH, New Delhi, 1972.

CH 002 : Preparatory Chemistry II **3 2 0**

Inorganic Chemistry

Periodicity in Properties: Ionization potential, electron affinity, ionic radii and electronegativity. Chemical Bonding: Ionic solids, Born-Haber cycle, covalent bonds, dipole moment, resonance, hybridization, geometry and shape of simple molecules. Coordinate Bond, Hydrogen bond.

Chemistry of p-block and d-block elements: Halogens; Periodicity of properties, preparation and uses of halogens and hydrogen halides. Oxides and oxyacids of chlorine.

Introduction to transition elements; oxides and oxyacids of sulphur, nitrogen and phosphorus.

Isolation of Metals; Extraction of Mg, Al, Zn, Cu and Fe.

Preparation and Properties of chemical compounds of industrial importance : Caustic soda, sodium carbonate, bleaching powder, superphosphate, gypsum alum, aluminium, chloride. Copper sulphate,silver nitrate, ammonia and ammonium sulphate.

Organic Chemistry

Classification and nomeclature of compounds. Empirical and molecular formula determination, isomerism. Electronic effects, resonance and inductive effects. Acidity of carboxylic acids and phenols, basicity of amines.

Covalent bond, types of hybridization in carbon compounds. Heterolysis and homolysis of covalent bonds - nucleophiles and electrophiles. Reactions of alkanes, alkenes and alkynes.

Characteristic reactions of common functional groups like alcohols, aldehydes, ketones, acids, esters and amines.

Difference between aliphatic annd aromatic compouds. Benzene and electrophilic substitution.

Text/References

R. T. Morrison and R. N. Boyd*, Organic Chemistry*, 6th edition, Pearson Com., 1992

P. Volhardt and N. Schore, *Organic Chemistry: Structure and Function*, 5th edition, W. H Freeman & Co, 2006

J. D. Lee*, Concise Inorganic Chemistry*, 4th edition, ELBS, 1991.

F. A. Cotton, G. Wilkinson, P. G. Gans, *Basic Inorganic Chemistry*, 2nd edition, John Wiley & Sons, 1987.

CH-011 : Preparatory Chemistry Laboratory I **0 0 3**

Practical exercises :

Experiments related to -

1. Acid-base titration.
2. Redox titration
3. Chemical Equilibrium
4. Ionic Equilibrium
5. Solubility Product
6. Chemical kinetics
7. Electrochemistry

CH-012 : Preparatory Chemistry Laboratory II **0 0 3**

1.Qualitative analysis of anions and cations.

2. Detection of elements- N, S, halogens
3. Separation and purification methods.
4. Melting point and boiling point determination.

CH 103 Chemistry - I **2 1 0 6**

Schrodinger equation (origin of quantization), Born interpretation of wave function, Hydrogen atom: solution to Φ-part, MO theory: atomic and molecular orbitals, Structure, bonding and energy levels of diatomic molecules. Examples N2, O2, CO and HF, Configuration, molecular chirality and isomerism, Conformation of alkanes and cycloalkanes, Reactivity of carbonyl group (addition reactions, reactions due to acidic proton, addition-elimination reactions and reactivity of acid halide, ester and amide), Functional group interconversions involving oxidation and reduction, Periodic properties: trends in size, electron affinity, ionization potential and electronegativity, Use of Ellingham diagram and thermodynamics in the extraction of elements, Transition metal chemistry: inorganic complexes, bonding theories, magnetism, bonding aspects and structural distortion, Bioinorganic chemistry: storage and transport proteins, Catalysis: hydrogenation, hydroformylation and olefin metathesis.

Text / References

P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, Oxford University Press, 8th edition, 2006.
I. N. Levine, *Physical Chemistry*, 5th edition, Tata McGraw-Hill, New Delhi, 2002.
D. A. McQuarrie and J.D. Simon, *Physical Chemistry - a molecular approach*, Viva Books Pvt. Ltd. (1998).
P. Volhardt and N. Schore, *Organic Chemistry: Structure and Function*, 5th Edition, W. H Freeman & Co, 2006
T. W. G. Solomons, C. B. Fryhle, *Organic Chemistry*, 9th Edition, Wilely India Pvt. Ltd., 2009
R. T. Morrison and R. N. Boyd*, Organic Chemistry*, 6th edition, Pearson Com., 1992
L. G. Wade*, Organic Chemistry*, Pearson Education 6th edition, 2006.
M. J. Sienko and R. A. Plane, *Chemical Principles and Applications*, McGraw Hill, 1980.
J. D. Lee, *Concise Inorganic Chemistry*, 4th Edition, ELBS, 1991.
D. D. Ebbing, *General Chemistry*, Houghton Miffin Co., 1984.

CH 104 Chemistry-II **2 1 0 6**

Chemical potential, Fugacities, activities, equilibrium constant, standard potential, Nernst equation, cell potential, concentration cells and applications, Chemical kinetics: steady state approximation, collision theory, Reaction mechanisms, energies and kinetics, Reaction types (nucleophilic, electrophilic, free radical reactions, polymerization reactions involving aliphatic and aromatic substrates), Molecular rearrangements Synthetic polymers and proteins, VSEPR theory, structure of boranes

and carboranes and electron counting, Inorganic rings, Metal carbonyls (synthesis, structure, bonding and reactivity), Organometallic reagents, Magnetism and superconductivity, Bioinorganic chemistry, activation and fixation of inert molecules.

Text / References

P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, Oxford University Press, 8th edition, 2006.
G. M. Barrow, *Physical Chemistry*, 5th edition, Tata McGraw-Hill, New Delhi, 1992.
D. A. McQuarrie and J. D. Simon, *Physical Chemistry - a molecular approach*, Viva Books Pvt. Ltd. (1998).
P. Volhardt and N. Schore, *Organic Chemistry: Structure and Function*, 5th Edition, W. H Freeman & Co, 2006
T. W. G. Solomons, C. B. Fryhle, *Organic Chemistry*, 9th Edition, Wilely India Pvt. Ltd., 2009
R. T. Morrison and R. N. Boyd*, Organic Chemistry*, 6th edition, Pearson Com., 1992
L. G. Wade, *Organic Chemistry*, Pearson Education 6th edition, 2006.
M. J. Sienko and R. A. Plane, *Chemical Principles and Applications*, McGraw Hill, 1980.
J. D. Lee, *Concise Inorganic Chemistry*, 4th edition, ELBS, 1991.
D. D. Ebbing, *General Chemistry*, Houghton Miffin Co., 1984.

CH 117: Chemistry Lab -I **0 0 3 3**

Experiments illustrating the concepts of 1) galvanic cells, (2) thermochemistry, (3) chemical kinetics, (4) equilibrium constant, (5) analysis by oxidation reduction titration.

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,* 6th edition, Saunders College Publisher, 1994.
G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denny, *Vogel's Text book of Quantitative Chemical Analysis*, 5th edition, ELBS, 1991.

CH 210 Inorganic Chemistry I **2 1 0 6**

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.

CH 211 Physical Chemistry-I **2 1 0 6**

Thermodynamic functions; Partial molar quantities; Phase rule, phase equilibria and applications; Non-ideal solutions; Mixing and excess functions; Chemical equilibria. Electrochemistry of solutions: Ion-solvent interactions; ion-ion interactions; ionic migration and diffusion.

Text / References

L. I. Antrapov, *Theoretical Electrochemistry*, Mir Publishers, 1972.
J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry, Vol. 1*, 2nd edition, Plenum Press, 1998.
P. Atkins and J. de Paula, *Atkins' Physical Chemistry*, 8th edition, Oxford University Press, 2006.
G. W. Castellan, *Physical Chemistry*, 3rd edition, Addison - Wesley/Narosa Publishing House, 1993.
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 221 Organic Chemistry-I **2 1 0 6**

Systematic study of structure, properties and chemistry of hydrocarbons with emphasis on theoretical, stereochemical and mechanistic concepts.

Text/References

P. Volhardt and N. Schore, *Organic Chemistry: Structure and Function*, 5th Edition, W. H Freeman & Co, 2006

T. W. G. Solomons, C. B. Fryhle, *Organic Chemistry*, 9th Edition, Wilely India Pvt. Ltd., 2009

R. T. Morrison and R. N. Boyd*, Organic Chemistry*, 6th edition, Pearson Com., 1992

CH 222 Organic Chemistry -II **2 1 0 6**

Prerequisite : CH 221

Chemistry of heterofunctional organic compounds. Systematic Study of structure, properties and chemistry of heterofunctional organic compounds with emphasis on theoretical, stereochemical and mechanistic concepts.

Text/Reference

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

P. Volhardt and N. Schore, *Organic Chemistry: Structure and Function*, 5th Edition, W. H Freeman & Co., 2006

T. W. G. Solomons, C. B. Fryhle, *Organic Chemistry*, 9th Edition, Wilely India Pvt. Ltd., 2009

R. T. Morrison and R. N. Boyd*, Organic Chemistry*, 6th Ed, Pearson Com., 1992

CH 316 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 317 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.

Texts/References

R. M. Roberts, J. C. Gilbert, L. B. Rodeward and A. S. Wingrove, *Modern Experimental Organic Chemistry*, Holf-Saunders Intnl. Edn., 4th edition, 1985.

CH 318 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 402 Thermal and Photochemical Reactions **2 1 0 6**

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 proceses. Electrocyclic reactions of cations, anions, radicals and radicals 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 perselectivity 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. Hammet 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 prepara- tions 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. Collison 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.Merrit, 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 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 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 H_2 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 **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 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 review 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 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 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 Analyis 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 ^{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 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^+, Mg^{2+} and Ca^{2+}. 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. Valentime, *Bioinorganic Chemistry*, Univ. Sci. Books, Mill Valley, 1994.
J. A.Cowan, *Inorganic Biochemistry*, VCH Publishers, 1993.
J. Reedijk, *Bioorganic Catlysis*, 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 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 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, antipsdychotics, antiinflammatory agents, cardiovascular agents, diuretics, antibacterials, antibiotics, antivirals, antimalarials, antiamoebics, 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 Gisveld'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, gentic code and protein synthesis. Enzymes-categorization, catalysis, kinetics-single substrate enzyme catalyzed reactions, inhibition. Lipids-structure and prop- erties of different classes of lipids. Biomembrane organisation-membrane lipids. Membrane bound proteins-structure, properties and transport phenomena. Bioenergetics-basic principles, glycolytic pathways, Kreb'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, 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. 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.

CH 552 Interfacial Phenomena **2 1 0 6**

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.

CH 556: Polymer Science **2 1 0 6**

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 Chemisty*, 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

CH 557 Topics in Chemistry **3 0 0 6**

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 Chemisty*, 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, 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-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 alkyla- tion, 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-595 : Project **0 1 10 12**

CH-596 : Project **0 1 16 18**