BHARATHIDASAN UNIVERSITY, TIRUCHIRAPPALLI 620 024
M.Phil. CHEMISTRY (FT/ PT) Programme
(For the candidates admitted from the academic year 2007-2008 onwards)

COURSE STRUCTURE

SEMESTER – I

	COURSE TITLE	MARKS			CREDITS
		IA	UE	TOT	
COURSE–I	Research Methodology and Laboratory Techniques	25	75	100	4
COURSE– II	Physical Methods in Chemistry I	25	75	100	*4*
COURSE– III	Physical Methods in Chemistry II	25	75	100	4

SEMESTER - II

COURSE–IV	ELECTIVE – (Any one) 1.Modern Methods of Organic Synthesis 2.Bioinorganic Chemistry 3. Principles and Applications of Organometallic Chemistry of Transition Metals 4.Principles and Advances in Medicinal Chemistry 5.Photophysics and Photochemistry 6 Molecular Modeling and Chemo & Bioinformatics 7. Nanochemistry	25	75	100	4
	Dissertation and Viva-Voce Viva Voce 50 marks Dissertation 150 marks			200 (150+50)	8

QUESTION PAPER PATTERN (Paper I – IV)

Part A : Two questions from each unit (without choice). Each question Carries marks (10 x 2 = 20)

Part B : One "EITHER OR" questions from each unit. Each question carries marks (5 x 5 = 25)

Part C : One question from each unit. Each question carries 10 marks. The candidate has to answer three questions out of the five questions (3 x 10 = 30)

BHARTHIDASAN UNIVERSITY, TIRUCHIRAPPALLI 620 024

M. Phil. CHEMISTRY

(For the candidates admitted from the academic year 2007-2008 onwards)

Paper 1: Research Methodology and Laboratory Techniques

UNIT I

1. Literature Survey

Web search and web publishing – Literature survey using internet – Web resources – Journal access through web – Digitized and digital formats – E-journals – e-Journals Consortium – UGC-Infonet – E-books – Online and Digital libraries – Useful web links – Search engines Alta vista, Google, Yahoo search – Wikis – Scifinder – Scopus – Scirus – Science Direct – Citation index – Iimpact factor – H-index – Internet discussion groups and communities – Blogs – Preprint servers – Sharing documents online – Report writing using templates – Correcting and editing on the web – Online submission system -- Tracking manuscript status – End-note and Sciproof – Digital object identifier – Hot articles.

UNIT II

2. Error Analysis

Types of Error – Accuracy, precision, significant figures, use of calculus in the estimation of errors – Frequency distributions, the binomial distribution, the Poisson distribution and normal distribution – Describing Data, population and sample, mean, variance, standard deviation, way of quoting uncertainty, robust estimators, repeatability and reproducibility of measurements – Hypothesis testing, levels of confidence and significance, test for an outlier, testing variances, means t-Test, Paired t-Test – Analysis of variance (ANOVA) – Correlation and Regression – Curve fitting, Fitting of linear equations, simple linear cases, weighted linear case, analysis of residuals – General polynomial equation fitting, linearizing transformations, exponential function fit – r and its abuse – Multiple linear regression analysis, elementary aspects – Applications of some computer packages like MS-Excel, Origin.

UNIT III

3. Instrumental Methods of Analysis

Basic aspects of synchronous fluorescence spectroscopy – Spectral hole burning – flow cytometry – Instrumentation on fluorescence ratio – Fluorimeters (quantization).

Structural methods: Extended X-ray absorption fine structure (EXAFS) – Surface extended X-ray absorption (SEXAFS). Operation modes of lasers – types of lasers - physical applications of lasers: on-linear optical effects-laser induced fluorescence – laser Raman spectroscopy, Atmospheric laser applications-laser systems as remote sensors-recent advances in analytical laser spectroscopy: Isotope analysis, Small molecules and radicals with pulsed lasers, Coherent anti-Stokes Ranab spectroscopy (CARS).

UNIT IV

4. Chromatography and Separation Techniques

Solvent extraction – Principles of ion exchange, paper, thin layer and column chromatography – Gas Chromatography techniques – Columns, adsorbents, methods, R_f values, McReynold's constants and their uses – HPTLC, HPLC techniques – Adsorbents, columns, detection methods, estimations, preparative column – GC-MS techniques: methods, principles and uses.

Electrophoresis: Principles, factors affecting ionic migration – Effect of pH and ionic strength – Gel electrophoresis.

UNIT V

5. Electroanalytical Techniques

Linear sweep voltammetry – Cyclic Voltammetry – Reversibility, elucidation of reaction mechanisms – Differential pulse voltammetry – Potentiometric stripping analysis – Chronocoulometry – Chronopotentiometry – Electrochemical sensors, ion-sensitive electrodes, glass-membrane electrodes, solid-liquid membrane electrodes - Ion-selective field effect transistors (ISFETs) – Sensors for the analysis of gases in solution – Amperometric gas sensors.

6. Electroorganic Synthesis

Electrophoresis: Principles, factors affecting ionic migration – Effect of pH and ionic strength – Gel electrophoresis.

References

UNIT I

1. http://www.virtualref.com/govdocs/s189.htm
2. http://www.inflibnet.ac.in
3. http://www.springerlink.com
4. http://rsc.org
5. http://www.pubs.acs.org
6. http://dspace.org
7. http://dspace.bdu.ac.in

UNIT II

1. D. B. Hibbert and J. J. Gooding, Data Analysis for Chemistry, Oxford University Press, 2006.
2. J. Topping, Errors of Observation and Their Treatment, Fourth Edn., Chapman Hall, London, 1984.
3. S. C. Gupta, Fundamentals of Statistics, Sixth Edn., Himalaya Publ. House, Delhi, 2006.
4. H. E. Solbers, Inaccuracies in Computer Calculation of Standard Deviation, Anal. Chem. **55,** 1611 (1983).
5. P. M. Wanek et al., Inaccuracies in the Calculation of Standard Deviation with Electronic Calculators, Anal. Chem. **54**, 1877 (1982).

UNIT III

1. A. Sharma, S. G. Schulman, Introduction to Fluorescence Spectroscopy, Wiley-Interscience, New York, 1999.
2. F. Rouessac and A. Rouessac, Chemical Analysis, John Wiley and Sons, Chichester, 2000.
3. C. N. Banwell and E. M. McCash, Fundamentals of Molecular Spectroscopy, 4th edn., Tata McGraw-Hill, New Delhi, 1994.
4. Nicolo Omemetto, Analytical Laser Spectroscopy, Vol.50, John-Wiley and Sons, New York, 1979.

UNIT IV

1. R. Stock and C. B. F. Rice, Chromatographic Methods, Chapman and Hall, New York. , 1963
2. B. S. Furniss, A. J. Hannaford, P. W. G. Smith, a. R. Tatchell, Vogel's Text Book of Practical Organic Chemistry, 5th Edition, Pearson, New Delhi, 1989
3. V. K. Srivastava and K. K. Srivastava, Introduction to Chromatography, S. Chand & Co., New Delhi, 2nd edition, 1981.

UNIT V

1. C. H. Hamann, A. Hamnett and W. Vilelstich, Electrochemistry, Wiley-VCH, 1998.
2. A. J. Bard and L. F. Faulkner, Electrochemical methods – Fundamentals and Applications, 2nd Edn., Wiley-VCH, 1998.
3. A. C. Fisher, Electrode Dynamics, Oxford University Press, 1996.
4. J. Koryta and K. Stulik, Ion-Selective Electrodes, Cambridge University Press, 1983.
5. J. Janata, Principles of Chemical Sensors, Plenum Press, New York, 1989.

PAPER II: PHYSICAL METHODS IN CHEMISTRY – I

UNIT I

1. Electronic Absorption Spectroscopy

Principles of absorption spectroscopy – Chromophore – UV-Visible Spectroscopy – Application to organic compounds – Woodward–Fieser and Scott rules for conjugated dienes and polymers – Ketones, aldehydes, α,β-unsaturated acids, esters, nitriles, and amides. Woodward's rule for enones – Differentiation of geometrical isomers and positional isomers – Disubstituted benzene derivatives – Study of steric effect on aromaticity.

Microstates – Term symbols and energy levels for d^1 – d^9 ions in cubic and square fields – Intensity of bands – Group theoretical approach to selection rules – Effects of distortion and spin-orbit coupling on spectra – Evaluation of 10dq and β values for octahedral complexes of cobalt and nickel – Applications to simple co-ordination compounds – Charge transfer spectra.

UNIT II

2. Infrared Spectroscopy

Vibrations in simple molecules (H_2O, CO_2) and their symmetry notation for molecular vibrations – Group vibrations and the limitations – Combined uses of IR and Raman Spectroscopy in the structural elucidation of simple molecules like N_2O, ClF_3, NO_3^-, ClO_4^- – Effect of coordination on ligand vibrations – Uses of group vibrations in the structural elucidation of metal complexes of urea, thiourea, cyanide, thiocyanate, nitrate, sulphate and dimethyl sulfoxide – Effect of isotopic substitution on the vibrational spectra of molecules – vibrational spectra of metal carbonyls with reference to the nature of bonding, geometry and number of C-O stretching vibrations (group theoretical treatment).

The modes of stretching and bonding – FT-IR – Sampling techniques – Correlation tables for functional groups – Alkanes, alkenes, alkynes, aromatic rings, alcohols, carbonyl compounds – Factors that influence C=O stretching vibration – Hydrogen bonding (inter, intramolecular).

3. Raman Spectroscopy

Theory – Selection rule – Mutual exclusion principle – Structural elucidation – Application to organic compounds – Factors affecting vibrational frequencies – Finger print region – functional groups and their characteristic vibrations – Resonance Raman Spectroscopy.

UNIT III

4. Optical Rotary Dispersion and Circular Dichroism

ORD and CD – Cotton effect – Octant rule, alpha-haloketone rule – applications to determining absolute configuration of simple monocyclic ketones and metal complexes.

5. Photoelectron Spectroscopy

Principles – Auger Electron spectroscopy – Electron spectra for chemical analysis.

6. Mass Spectrometry

Instrumentation – Resolution, EI and CI methods – base peak, isotopic peaks, metastable peak, parent peak – determination and use of molecular formula, recognition of molecular ion peak – FAB – Fragmentation – General rules – Pattern of fragmentation for various classes of compounds – McLafferty rearrangement – Importance of metastable peaks – Inorganic Applications – Molecular fragmentations – Ion reactions.

UNIT IV

7. Diffraction Methods

Crystal symmetry – combination of symmetry elements – crystal classes – screw axis and glide planes – space group – crystal axes - crystal systems, unit cell, Bravois lattices, asymmetric unit – space group – Equivalent positions – X-ray diffraction by single crystals – Structure factor – Phase problem in structure analysis – Heavy atom method – Fourier synthesis – refinement of structure.

Neutron diffraction – Applications and comparison with X-ray diffraction.

Electron diffraction by gases – Basic principles and applications to simple molecules – XeF_6, $Be(Bh_4)_2$, ferrocene, Cr(II) acetate.

UNIT V

8. Techniques in Nano Chemistry

Techniques for Characterization of nanoscale materials (Basic aspects): Atomic force microscopy (AFM) – Transmission electron microscopy (TEM) – Resolution and scanning transition electron microscopy (STEM). Scanning Tunneling Microscopy (STM) – Scanning nearfield optical microscopy (SNOM) and surface plasmon spectroscopy.

References

UNIT I

1. A. B. P. Lever, Inorganic Electronic Spectrosopy, American Elsevier, 1968, 1986.
2. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern company

UNIT II

1. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern company.
2. N. B. Clothup, L. H. Daly and S. E. Wiberly, Introduction to Infrared and Raman Spectroscopy, Academic Press, New York, 1975.
3. R. S. Drago, Physical Methods in Chemistry, W. B. Saunders company, Philadelphia, London.
4. D. N. Sathiyanarayana, Vibrational Spectroscopy, New Age International Publishers, New Delhi.
5. K. Nakamoto, Infrared Spectra of Inorganic and Coordination Compounds, 2nd Ed, Wiley-Inter Science, New York.
6. D. L. Pavia, G. M. Lampmann, G. S. Kriz, Introduction to Spectroscopy, Thomson, 3rd edition, 2001.

UNIT III

1. J. E. Eland, Photoelectron Spectroscopy, Wiley, 1974.
2. P. K. Ghosh, Introduction to Photoelectron Spectroscopy, John wiley and sons, New York, 1983.
3. D. L. Pavia, G. M. Lampmann, G. S. Kriz, Introduction to Spectroscopy, Thomson, 3rd edition, 2001.

UNIT IV

1. P. J. Wheatley, The Determination of Molecular Structure, (Unit V).
2. E. A. V. Ebsworth, David W. H. Rankin and Stephen Cradock , Structural Methods in Inorganic Chemistry, Blackwell Scientific Publications, U. K. 1987.

UNIT V

1. Kenenth J. Klabunde (Ed), Nanoscale Materials in Chemistry, Wiley - Interscience, New York, 2001.
2. T. Pradeep, Nano: The Essentials in Understanding Nanoscience and Nanotechnology, Tata McGraw Hill, New Delhi, 2007.
3. Willian Clegg, Crystal Structure Determination, Oxford University Press, 1998.

PAPER III: PHYSICAL METHODS IN CHEMISTRY – II

UNIT I

1. NMR Spectroscopy: Principles

Definition of nuclear angular momentum and the nuclear magnetic moment : Idea about the rotating axis system – Bloch equations – Quantum mechanical description of the NMR experiment, transition probabilities – Relaxation effects – Fourier transform NMR – Measurement of T_1 and T_2 . Effect of quadrupolar nuclei- evaluation of thermodynamic and kinetic data using NMR techniques – Second order spectra – Quantum mechanical treatment of coupling effects of relative magnitudes of J on the spectrum of an AB molecule - Spectral simplification and determination of signs of coupling constants.

Systems with chemical exchange – Evaluation of thermodynamic parameters in simple systems – Study of fluxional behaviour of molecules an elementary treatment of second order spectra – examples.

2. NMR Spectroscopy: Applications to Inorganic Systems

^{1}H, ^{19}F, ^{31}P, ^{13}C – Applications in probing inorganic structures, study of fluxional behaviour in organometallics,evaluation of thermodynamic parameters – NMR of paramagnetic molecules – isotropic shifts – Contact and pseudo-contact shifts – Lanthanide shift reagents.

UNIT II

3. NMR Spectroscopy: Proton and Carbon NMR

Examples for different spin systems – Chemical shifts and coupling constants (Spin-spin coupling) involving different nuclei (^{1}H, ^{19}F, ^{31}P, ^{13}C) – interpretation and applications to inorganic compounds – Effect of quadrupole nuclei (^{2}H, ^{10}B, ^{11}B) on the proton NMR spectra – Satellite spectra.

^{1}H NMR Spectroscopy – Coupling constant – First order and second order splitting – Spin-spin splitting – Dependence of J on dihedral angle – Vicinal and geminal coupling constants – Karplus equation – Long range coupling constants - Influence of stereochemical factors on chemical shift of protons – Simplification of complex spectra – Double resonance techniques – Shift reagents – Chemical spin decoupling of rapidly exchangeable protons (OH, SH, COOCH, NH, NH_2) – An elementary treatment of NOE phenomenon – 2D Techniques (COSY, NOESY and ROSY)

4. Application of Proton NMR in MRI

^{13}C NMR spectroscopy – Basic theory of FT-NMR – Relaxation – Broad band decoupling – Off resonance decoupling and chemical shift correlations (CH, CH_2, CH_3, aromatic). Identification of structure based on NMR data – Problems.

UNIT III

4. NQR Spectroscopy

Introduction – Characteristics of quadrupolar nuclei – Effects of field gradient and magnetic field upon quadrupolar energy levels – NQR transitions – Applications of NQR spectroscopy.

5. Mössbauer Spectroscopy

Introduction – Isomer shift – Magnetic interactions – Mössbauer emission spectroscopy – Applications to iron and tin Compounds.

UNIT IV

6. Electron Spin Resonance Spectroscopy

Basic concepts of ESR spectroscopy – Spin densities and McConnell equation – Hyperfine splitting –Factors affecting the magnitude of g and A values – Anisotropy in g and A values – ESR spectra of free radicals in solution: methyl, allyl, vinyl and related radicals, benzene anion, p-benzo-semiquinone, p-nitrobenzoate dianion – naphthalene dianion, – Spin-trapping – CINDNP and CIDEP techniques – Double resonance in ESR – Advantages of ENDOR spectroscopy.

UNIT V

7. Electron Paramagnetic Resonance Spectroscopy

Applications of EPR to some simple inorganic systems such as Xe_2^+ – Factors affecting the magnitude of g and A tensors in metal complexes – Zero-field splitting and Kramers degeneracy – Spectra of VO(II), Mn(II), Fe(II), Co(II), Ni(II) and Cu(II) complexes – EPR spectra of dinuclear Cu(II) complexes - Applications of EPR to a few metallobiomolecules containing Cu(II) and Fe(III) ions.

Basic principles of ENDOR spectroscopy and its applications in inorganic Chemistry.

References

UNIT I

1. E. A. V Ebsworth, David W. H. Rankin and Stephen Cradock, Structural Methods in Inorganic Chemistry, Blackwell Scientific Publications, U. K. 1987

UNIT II

1. W. Kemp, NMR in Chemistry – A Multinuclear Introduction, McMillan, 1986.
2. C. D .Becker, High Resolution NMR – Theory andApplications, Academic Press, 2nd Edition, 1980.
3. Silverstein and Webster, Spectrometric Identification of Organic Compounds, Sixth Edition, Wiley, 1998.
4. B. P. Straughan and S. Walker , Spectroscopy Vol. I, Chapman and Hall, 1976.
5. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Edition, Wiley Eastern Company.
6. D. L. Pavia, G. M. Lampmann, G. S. Kriz, Introduction to Spectroscopy, Thomson, 3rd edition, 2001.

UNIT III

1. R. S. Drago, Physical Methods in Inorganic Chemistry, 3rd Ed., Wiley Eastern company.
2. T. C. Gibbs, Principles of Mössbauer Spectroscopy, Chapman and Hall, 1976.
3. T. P. Das and E. L. Hah, NQR Spectroscopy, Acad. Press, Ny, 1958.

UNIT IV

1. B. P. Straughan and S. Walker, Spectroscopy, Chapman and Hall, London, vol.1 and 2, 1976.
2. C. N. Banwell, Fundamentals of Molecular Spectroscopy, 3rd edition, Tata-McGraw Hill, New Delhi, 1983.

3. G. M. Barrow, Introduction to Molecular Spectroscopy, McGraw-Hill,New York, 1964.
4. R. S. Drago, Physical Methods in Chemistry, Saunders, 1977.

UNIT V

1. R. S. Drago, Physical Methods in Inorganic Chemistry, Third Edition, Wilely Eastern,
2. M. C. R. Symons, Chemical and Biochemical Aspects of Electron Spin Resonance Spectroscopy, Van Nostrand Reinhold Co., 1978.
3. J. A. Weil, J. R. Boldton and J. E. Wertz, Electron Paramagnetic Resonance: Elementary Theory and Practical Applications, John Wiley and sons, 1994.
4. F. E. Mabbs and D. Collison, Electron Paramagnetic Resonance of d Transition Metal Compounds, Elsevier, 1992.

Paper - IV: ELECTIVE PAPER

1. Modern Methods of Organic Synthesis

UNIT I

1. Synthons and Synthetic Equivalents

Introduction to disconnections – Synthons and synthetic equivalents – Electron donors (nucleophiles) – electron synthon approach – Electron acceptors – (electrophiles) – Introduction of functional groups – Rregioselective and stereoselective alkylation of cyclic ketones, cyclic enones.

C-alkylation versus O-alkylation: Enamines and selection alkylation (Mono and di) via enamine reactions. Olefination of carbonyl compounds – Wittig reactions, McMurry method.

2. Retrosynthetic Analysis of Simple Organic Compounds

Antithesis of mono and dofunctional open chain target molecules. Retrosynthetic analysis of monocyclic and bicyclic target molecules.

UNIT II

3. Reagents for Reduction and Oxidation

Catalytic hydrogenation and dehydrogenation, Reduction with LAH, $NaBH_4$, Tritertiarybutoxy aluminum hydride, $NaCNBH_3$, Tributyltin hydride, Me_3SiCN, Alkali metals for reduction, Reductions with hydrazines. Osmium tetroxide, Sharpless asymmetric epoxidation, Chromyl chloride, Ozone, DDQ, Dioxiranes, Lead tetraacetate, Selenium dioxide, DMSO either with Ac_2O or Oxalyl chloride, Dess-Martin reagent. LDA, Phase transfer catalysis (PTC), Merrifield resin, Baker's yeast

4. Functional Group Interconversions

Modern methods of functional group interconversion involving C=O, CHO, -OH, -SH, -COOH, C=C, NH2, COOR, CONHR functions. Reversible protection of reactive sites.

UNIT III

5. Asymmetric Synthesis

Introduction: Basic principles of Asymmetric synthesis – Definition – Stereospecific, Stereoselective – Enanatioselective and diastereoselective.

Asymmetric synthesis using chiral reagents: Chiral organoboranes – Application of chiral organoboranes, Reduction (Ipc_2BCl) and allylation and crotylation reactions, T.S. models; Chiral modification of lithium aluminum hydride, BINAL-H – Application in reduction of prochiral ketones; Oxazaborolidines. T.S. model.

Asymmetric synthesis using chiral auxiliary: Chiral auxiliaries derived from proline, Champhor, Menthol and Other chiral pool sources.

Asymmetric synthesis using chiral catalysts: Asymmetric alkylation and allylation of carbonyl compounds, Chirality amplification: Selected reactions: Keck's allylation, TADDOLs and other privileged ligands.

Asymmetric hydrogenation: Early advances DIPAMP, DIOP and Noyori's BINAP. Jacobson catalyst – Evans catalyst.

UNIT IV

6. Transition Metals in Organic Synthesis

Formation of C-C single bonds: Organolithium reagents, Organomagnesium reagents, Organozinc reagents, Application of Organocopper, Organochromium, Organocobalt and Organopalladium chemistry.
Formation of C-C double bonds: Alkene metathesis reactions using ruthenium complexes.

UNIT V

7. Green Chemistry

Definition, principles and evolution of green chemistry. Heterogeneous reaction for green chemistry. Alternative solvents: ionic liquids, super critical fluid extraction, organic synthesis using water resistant Lewis acids. Solvent free reaction: Microwave assisted organic synthesis-the reaction vessel, medium, advantages, limitations and application. The use of ultrasound in organic synthesis: Introduction, instrumentation, types of sonochemical reactions, esterification, substitution, oxidation, reduction.

Textbooks and Reference books

1. R. K. Mackie and D. M. Smith, Guide Book to Organic Synthesis ELBS, 1982.
2. S. Waver, Organic Synthesis, The disconnection approach, John Wiley & Sons, 1982.
3. J. March, Advanced Organic Chemistry : Reactions, Mechanisms and Structure, 5th ed., Wiley, 1996.
4. S. H. Pine, J.B. Hendrickson, D. J. Cram and G. S. Hammond, Organic Chemistry, McGraw Hill, 4th ed., 1980.
5. T. H. Lowry and K.S. Richardson, Mechanism and Theory in Organic Chemistry, Harper and Row, 1976.
6. J. D. Morrison, Asymmetric Synthesis: Vol 1-5, Academic Press, 1983.
7. E. N. Jacobsen, A. Pfaltz,. H. Yamamoto, Eds., Comprehensive Asymmetric Catalysis, Springer 2000.
8. R. Noyori,.Asymmetric Catalysis in Organic Synthesis, Wiley-NY 1994.
9. I. Ojima, Catalytic Asymmetric Synthesis , VCH-NY, Pergamon, 1998.
10. H. B. Kagan, Aymmetric Synthesis, Thieme Medical Publishers, Ist Edn., 2003.
11. W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, Cambridge University Press, 4th edition, 2004.
12. I. L. Finar, Organic Chemistry, Vol.II, 5th ed., ELBS, 1975.

13. P. T. Ananstas, J.C.Warner, Green chemistry- Theory and practice, Oxford University press New York, 2000.
14. R. Sanghi, M. M. Srivastava Narosa, Green chemistry- Environment friendly Alternatives, Publishing house, Chennai 2003.
15. V. K. Ahluvalia, R. Agarwal, Narosa Publishing house, Organic synthesis- Special techniques, Chennai 2001.

2. Bio-Inorganic Chemistry

UNIT I

1. General Principle

Occurrence and availability of inorganic elements in organisms – Biological function of inorganic elements – Biological ligands for metal ions – Coordination of Proteins and enzymatic catalysis – Porphyrins and other Macrocylces – Other metal binding molecules like Prosthetic groups, coenzyme B_{12}, bleomycin and siderophores – Communication roles for metals in biology.

Proteins and their constituents – Nucleic acids and their constitutents.

Biological functions of boron, silicon, arsenic, phosphine, bromine, fluorine, iodine and selenium.

2. Function and Transport of Alkali and Alkaline Earth Metal Ions

Characterization of K^+, Na^+, Ca^{2+} and Mg^{2+} complexes of alkali and alkaline earth metal ions with macrocycles – Ion channels – ion pumps – Catalysis and Regulation of bioenergetic processes by the alkaline earth metal ions Mg^{2+} and Ca^{2+}. Uptake, transport and storage of Iron – Siderophores phytosiderophores – transferrins – Ferritin.

3. Biomineralisation

Biomineralisation – Nucleation and crystal growth – various biominerals – calcium phosphate – calcium carbonate – Iron biominerals.

UNIT II

4. Cobalamines

History and structural characterization – Reactions of methylcobalamines – One-electron reduction and oxidation – Co-C Bond cleavage – Role of the apoenzyme.

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5. Metals at the Center of Photosynthesis

Volume and total efficiency of photosynthesis – Primary processes in photosynthesis – Light absorption – Exciton Transport – Charge separation and electron transport – Manganese catalysed oxidation of water to O_2.

UNIT III

6. Iron Proteins

Oxygen Transport through Haemoglobin and Myoglobin – Alternative oxygen transport in some lower animals: Hemereythrin and Hemocyanin. Electron transfer, oxygen activation and metabolism of Inorganic intermediates – Cytochromes – Cytochrome P450 – Haemoproteins in catalytic transformations.

7. Iron-sulfur and other Non-heme Iron Proteins

Classification – Rubredoxins – Ferredoxins – Model systems – Non-heme iron enzymes – ribonucleolide reductase (RR) – Methane monooxygerase (MMO) – Purple acid phosphatases – Mononuclear non-heme iron enzymes.

8. Copper Proteins

Classification and examples - Electron transfer – Oxygenation – oxidases and reductases – Cytochrome c Oxidase – Superoxide dismutase (Cu, Zn).

UNIT IV

9. 'Early' Transition Metals

Molybdenum – Metalloenzymes in the biological Nitrogen Cycle: Molybdenum – Dependent Nitrogen Fixation – Nitrogenases – Chromium(III) in metabolism.

10. Nickel Enzymes

Nickel containing Enzymes – Urease, Hydrogenases.

11. Zinc Enzymes

Carbonic anhydrase – Carboxypepsidase – The catalysis of condensation reactions – alcohol dehydrogenate – Zinc finger proteins – Insulin and Metallothionein.

UNIT V

12. Medicinal Bioinorganic Chemistry

Bioinorganic Chemistry of Quirtessentially toxic metals – Lead, Cadmium, Mercury, Aluminium, Chromium, Iron, Copper, Plutonium – Detoxification by metal chelation. Drugs which act by binding at the metal sites of Metalloenzymes.

13. Biochemical behaviour of Inorganic Radionuclides

Radiation risks and medical benefits – Natural and Manmade radioisotopes. Bioinorganic Chemistry of Radio pharmaceuticals – Technicium.

14. Chemotherapy

With compounds of certain non-essential elements – Platinum complexes in Carartherapy – Cisplatin and its mode of action – Cytotoxic compounds of other metals – Gold containing drugs as anti-rheumatic agents and their mode of action – Lithium in Pschycopharmocological drugs.

Text Books

1. James E. Huheey, Inorganic Chemistry, 3rd Ed, Harper & Row Publishers, Singapore.
2. Purcell and Kotz, Inorganic Chemistry, Saunders Golden Sunburst Series, W. B. Saunders Company, Philadelphia (Units III, IV & V)
3. Robert W. Hay, Inorganic Chemistry, (Unit I and III)
4. S. J. Lippard and J. M. Berg, Principles of Bioinorganic Chemistry, Panima Publishing Company, New Delhi, 1997.

5. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John Wiley & Sons, New York.
6. F. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, 5th Ed., Chem. A. Wiley, Interscience Publication, John-Wiley & Sons, USA.

Reference Books

1. Bioinorganic Chemistry, State of the Art , J. Chem., Education, 62, No. 11, 1985.
2. G. I. Eichhorn, Ed . Inorganic Biochemistry, Vols 1 & 2.

3. Principles and Applications of Organometallic Chemistry of Transition Metals

UNIT I

1. Structure and Bonding: Electronic Book Keeping

Electronic configuration of the transition metals – Oxidation state formalism – d-electron configuration and the 18 electron rule – Spatial orientation of d-orbitals - Molecular orbital description of octahedral complexes – Ligand field orbital splitting for various coordination geometries – Simplified electron counting scheme.

2. Survey of Organotransition Metal Complexes According to Ligand

Classic Lewis Base donors – Phosphine and other group VB donors – Hydrides - carbon bonded ligands –- End bound π-acid ligands – Side-bound π-acid carbon ligands – Unsaturated nitrogen ligands – dioxygen and its derivatives – Sulphur dioxide.

UNIT II

3. Oxidative Addition and Reductive Elimination Reactions

Oxidative addition reactions with an overall two electron change – reactions with protons – Reactions forming metal-carbon bonds – Planar Ir(I) complexes – d^{10} complexes – Macrocyclic Rh(I) complexes - Organo copper reagents – Alkylation of coorinatively saturated complexes – Acylation – Oxidative addition of H_2 – Oxidative addition with an overall one electron change – Mononuclear Reactions forming carbon-carbon bonds and carbon-Hydrogen bonds .

UNIT III

4. Insertion Reactions

Migratory insertions – Migrations to CO-migrations to other longitudinal ligands – Thiocarbonyls – isonitriles – carbenes – Migrations to olefins and acetylenes – Migratory insertions involving hydrides and olefins-migratory insertions involving metal alkyls and olefins or acetylenes – Nucleophillic attack on coordinated olefin, acetylene, arene, η^3-allyl, η^5-C_5H_5, carbyne.

UNIT IV

5. Homogeneous Catalytic Hydrogenation and Hydrosilation

Overview – Mechanism – General features of Wilkinson's catalyst – Mechanism of hydrogenation of Rh(I) catalyst – Asymmetric homogeneous hydrogenation – Other hydrogenation catalysts – Supported transition metal complex hydrogenation catalysts – Relative advantages of homogeneous versus heterogeneous hydrogenation catalysts – Homogeneously catalyzed hydrosilation.

UNIT V

6. Formation and Fragmentation of Metallacycles

Isolobal analogy – Structural implications of isolobal analogy – metallacyclobutanes – Metallacyclopentanes – Metallacyclopentadiene – Metallacyclopentenes.

Text Books and Reference Books

1. J. P. Collman and L. S. Hegedus, Principles and Applications of Organotransition Metal Chemistry,
   Oxford University Press, 1980.
2. R. Hoffman, Angew Chem., Int. Ed.(Eng) 21, 711 (1982)
3. R. H. Crabtree, The Organometallic Chemistry of the Transition Metals, John Wiley & Sons, New York.
4. I. Haiduc and J. J. Zuckermann, Basic Organometallic Chemistry.
5. P. Powell, Principles of Orgnanometallic Chemistry, 2nd, Chapman and Hall, London.

Prerequisites

1. F. A. Cotton and G. Wilkinson, Advanced Inorganic Chemistry, Interscience, 1980.
2. J. E. Huheey, Inorganic Chemistry, Harper and Row, 1978.

4. Principles and Advances in Medicinal Chemistry

UNIT I

1. Nomenclature and Mechanism of Drugs

Introduction – Study of drugs – Important terminologies in pharmaceutical chemistry – Classification and nomenclature of drugs – Nomenclature of some heterocyclic systems – Mechanism of action of drugs – metabolism of drugs – Absorption of drugs – Assay of drugs.

UNIT II

2. Drug Discovery and Development

Introduction – Choosing a drug target – Identifying a bioassay – Finding a lead compound – Structure-activity relationship(SAR) – Identification of a pharmacophore – Drug metabolism – Manufacture-synthetic issues – Toxicity – Clinical trials – Patents.

UNIT III

3. Drug Design and Pharmacokinetics

Drug design: Variation of substituents, chain extension, ring expansions/contractions, ring variations, ring fusions, isosteres, rigidification of the structure, conformational blockers.
Pharmacokinetics: Pharmacokinetics issues in drug design – Solubility and membrane permeability – Resistant to hydrolysis and metabolism – Targeting drugs – Reducing toxicity – Prodrugs – Methods of administration – Formulation.

UNIT IV

4. Combinatorial Synthesis

Introduction – Combinatorial synthesis for drug discovery – Solid phase techniques – Methods of parallel synthesis – Mixed combinatorial synthesis – Deconvolution – Structure determination of the active compound – Limitations – Examples – Designing a combinatorial synthesis – Testing for activity.

UNIT V

5. Application of Drugs for Treatment

Structure, properties and mechanism of action of the following: Antibacterial drugs – Sulpha drugs: Sulphanilamide, Sulphadiazine, Suphapyridine. Antibiotics – Chloramphenical, Pencillin, Streptomycin. Antiseptics and disinfectants: Phenol and its derivatives, Halogen compounds and organic mercurials. Analgesics: Morphine, Heroin, Pethidine, Morphinan. Anticonvulsant: Barbiturates, Oxazolindiones. Diabetes: Control of diabetes, Insulin. Cancer and antineoplastic drugs: Allylating agents, Antimetabolites, Plant products. Cardio vascular drugs: Antiarrhythemic drugs, Antihypertension drugs.

Textbooks and Reference books

1. G. L. Patrick, An Introduction to Medicinal Chemistry, Oxford University Press, 2nd Edition,
2001.
2. J. Ghosh, Fundamental Concepts of Applied Chemistry, S. Chand and Co., New Delhi, 2006.
3. A. Kar, Medicinal Chemistry, New Age International (P) Ltd, Delhi, 1997.

5. Photochemistry and Photophysics

UNIT I

1. Physical Properties of Electronically Excited Molecules

Nature of changes on electronic transition – Shapes of absorption band and Franck-Condon principle - Emission spectra - Environmental effect on absorption and emission spectra – Excited state dipole moment – Excited state acidity constants-pK values – Excited state redox potential – Emission of polarized luminescence – Geometry of some electronically excited molecules – Flash photolysis experiments.

UNIT II

2. Photophysical Processes and their Kinetics

Types of photophysical pathways – Radiationless transition (internal conversion and intersystem crossing)-Fluorescence emission – Fluorescence and structure – Triplet states and phosphorescence emission – Delayed fluorescence – Kinetic collisions and optical collision-kinetics of collision quenching : Stern- Volmer equation, concentration dependence of quenching and excimer formation.

UNIT III

3. Applied Inorganic Photochemistry

Some liquid-phase actinometers involving metal complexes, potassium ferrioxalate, uranyl oxalate, Reinecke's salt – Applications of Inorganic photo chemistry in the photochemical conversion and storage of solar energy, photochemical isomerization reactions, usefulness of photoredox reactions, photochemical cleavage of water into hydrogen and oxygen, uses of polypyridineruthenium(II) metal complexes – Natural and artificial photosynthesis – Photosynthetic apparatus and the two photo systems, chlorophylls, mechanism of electron transport, some model systems for reaction centres of natural photosynthesis.

UNIT IV

4. Photochemistry in Microheterogeneous Systems

Photophysics and photochemistry of substances in micelles, luminescence probe analysis of singlet and triplet states, dynamics of excimer and exciplex charge-transfer reactions, micellar cage effect – Reactions in reverse micelles and microemulsions, oil-in-water and water-in-oil type – Photoprocesses in lipids, surfactant vesicles and liposomes, general features of fluorescence quenching

analysis and excitation energy and electron transfer processes – Photoprocesses in monolayers, black lipid membranes and liquid crystalline solvents – Photoprocesses in polymers, polyelectrolytes and ion-exchange membranes – Photoprocesses in molecular inclusion complexes like cyclodextrins, zeolites etc.,

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UNIT V

5. Organic Photochemistry

Principles of photochemistry, Characteristics of photoreactions, Photoreduction and photoxidation and photoreactions of ketones and enones, Norrish Type I and II reactions. Photochemistry of alkenes, dienes and aromatic compounds reactions of unactivated centres – Photolytic cycloadditions and photolytic rearrangements – Photosenstitisation – Photoadditions – Barton reaction – Parterno Buchi reaction. Reactions with singlet oxygen.

Reference Books / Text Books

UNIT I and UNIT II

1. K. K. Rohatgi-Mukherjee, Fundamentals of Phtochemistry, Wiley Eastern Ltd., New Delhi, 1978.
2. B. P. Wayne,Photochemistry, Butterworths, London, 1970.
3. N. J. Turro, Molecular Photochemistry, W. A. Benjamin,New York, 1966.
4. R. P. Cundall and A. Gilbert, Photochemistry, Thomas Nelson, London, 1970.

UNIT III

1. A. W. Adamson and P. D. Fleischauer(Editors), Concepts of Inorganic Photochemistry, Wiley, New York, 1975.
2. G. J. Ferraudi, Elements of Inorganic Photochemistry, Wiley, New York, 1993.
3. D. O. Hall and K. K. Rao, Photosynthesis, Cambridge University Press, Cambridge, 1996.
4. J. Chem. Edn., Vol.60, Number 10, October 1983.

UNIT IV

1. K. Kalyanasundaram, Photochemistry in Microheterogeneous Systems, Academic Press, 1983.
2. J. Chem. Edn., Vol.60, Number 10, October 1983

UNIT V

1. C. H. Depuy & O. L. Chapman , Molecular Reactions and Photochemistry , Eastern economic edition, Tata Mc Grow Hill, 1975.
2. J. M. X. Coxon, B. Halton, Organic Photochemistry, Camb. Univ., 2nd edition, 1987.
3. G. R. Chatwal, Organic Photochemistry, 1st edition, Himalayan Publ. House, Mumbai, 1998.

6. Molecular Modeling and Chemo & Bioinformatics

UNIT I

1. Quantum Mechanics

Polyatomic molecules – quantum chemistry of a chemical bond – Molecular orbital description – the Hartree-Fock equation – Basis sets – Roothan-Hall equation – approximations and parameterizations – semi empirical methods and their performance – Hartree-Fock limit - electron correlation and post Hartree Fock methods – Configuration Interaction, perturbation and many body methods – Density Functional Theory (DFT) – Hohnberg-Kohn existence and variation theorems – Kohn Sham equations – LDA , NDA and Hybrid functionals – advantages and limitations of DFT

UNIT II

2. Molecular Mechanics

General feature of molecular mechanics and force fields – Bond stretching, bending, tensional terms – Non-bonded and electrostatic interactions- Vander-Walls interaction – Force field parameterization and its transferability – use of force fields in organic chemistry - force fields for inorganic molecules – Proteins and nucleic acids.

UNIT III

3. Molecular Dynamics

Introduction to molecular dynamics – Simple methods - continuous potentials – Finite difference and predictor – Corrector method – Verlet algorithm – Choosing the time steps – NVT and NPT dynamics. Stochastic dynamics

UNIT IV

4. Chemoinformatics

Computer representation of molecules – Chemical databases and 2D substructure searching - 3Ddata base searching – Similarity and similarity searching – Molecular descriptors – QSAR – Neural network – computational library – Application to drug design.

UNIT V

5. Bioinformatics

Fundamentals of protein and nucleic acid structure – Molecular visualization – Open access bibliographic resources and literature database: PUBMED, Biomed central and PLOS – Sequence database: GenBank, DDBJ & EMBL – PIR & SWISS –Port – Structure databases :PDB and NDB – principles and method of docking and ligand design – Method and tools – Free energy of binding – Scoring function – Test of methods

Reference Books

1. Andrew R Leach, Molecular Modeling: Principles and Applications, 2nd Edition, Prentice Hall, London 2001
2. Arthur M. Lesk, Introduction to Bioinformatics, Oxford University Press New Delhi, 2003.
3. A. Baxevanis and B. F Ouellette Bioinformatics: A Practical guide to the analysis of genes and proteins, Third edition, Wiley Inter Science, 2005
4. P. E Bourne, Structural Bioinformatics, H. Weissing (Eds), Wiley Liss, 2003 Chapters 2, 3, 7 and 22

2. Further Reading

1. Christopher J Cramer, Essentials of Computational Chemistry : Theories and Models, John Wiley, New York, 1961

2. Frank Jenson, Introduction to Computational Chemistry, Wiley, New York, 1999

7. Nanochemistry

UNIT – I

1. Nanochemistry – An Introduction

Definition of nanodimensional materials - Some historical milestones in the saga of nano forms - Size effects - Importance of Nanomaterials - Classification of Nanomaterials - Simple examples of unique properties of nanosized materials - Elementary aspects of bionanotechnology - Some important recent discoveries in nanoscience and technology.

UNIT – II

2. Techniques in Nanochemistry

Techniques for Characterisation of nanoscale materials (Basic aspects): Atomic force microscopy (AFM)-Transmission electron microscopy (TEM)-Resolution and scanning transmission electron microscopy (STEM) Scanning Tunneling Microscopy (STM) Scanning nearfield optical microscopy (SNOM) and surface plasmon spectroscopy.

3. Photochemistry and Electrochemistry of Nanoassemblies

Semiconductor nano particles – Photo-induced charge Tranfer processes – Electrochemistry of Semiconductors - Nano structures - Nanostructural Oxide films modified with dyes and redox chromophores - Electrochemistry of metal nano structures – Particles – Nanoclectrodes – Biosensors – Chemical sensors.

UNIT III

4. Biomineralisation

Biomineralisation - Controller assembly of advanced materials in Biology - Nucleation and crystal growth – Various biominerals – Calcium phosphate – Calcium carbonate – Amorphous silica, Iron biominerals – Strontium and barium sulphates.

5. Inorganic Nanoparticles and Nanoporous Materials

Oxide nano particles – Oxomolybdates – Nano catalysis – Porous silicon – Transition and Non transition metal phosphates.

UNIT – IV

6. Carbon Clusters and Nanostructures

Nature of carbon bond – New carbon structures – Carbon clusters: Discovery of C_{60} – Alkali doped C_{60} – Superconductivity in C_{60} – Larger and smaller fullerenes. Carbon nanotubes: Synthesis – Single walled carbon nanotubes – Structure and characterization – Mechanism of formation – Chemically modified carbon nanotubes – Doping – Functionalizing nanotubes – Application of carbon nanotubes. Nanowires – Synthetic strategies – Gas phase and solution phase growth – Growth control – Properties.

UNIT V

6. Organic Films and Supramolecular Assembly

Organic films - Insulating and passivating layers – Electron transfer – Organic nanostructures – Optical properties – Organic semiconductors – Active organic devices. Polymerization – Sizes of polymers – Nanocrystals – Conductive polymers – Block co-polymers. Supramolecular structures – Transition-metal-mediated types - Dendritic molecules – Supramolecular dendrimers – Micelles – Biological nanostructures – Examples of proteins.

References

1. C. N. R. Rao, A. Muller, A.K. Cheetam (Eds), The Chemistry of Nanomaterials, Vol.1, ao 2, Wiley – VCH, Weinheim, 2004.
2. C. P. Poole, Jr: F. J. Owens, Introduction to Nanotechnology Wiley Interscience, New Jersey, 2003
3. Kenneth J. Klabunde (Ed), Nanoscale materials in Chemistry, Wiley-Interscience, New York, 2001.
4. T. Pradeep, Nano: The Essentials in understanding nanoscience and nanotechnology, Tata McGraw Hill, New Delhi, 2007.
5. H. Fujita (Ed.), Micromachines as tools in nanotechnology, Springer- Verlag, Berlin, 2003.

6. Bengt Nolting, Methods in modern biophysics, Springer-Verlarg, Berlin, First Indian Reprint, 2004.
7. H. Gleiter , Nanostructured Materials: Basic Concepts, Microstructure and Properties
8. W. Kain and B. Schwederski, Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life, John- Wiley R Sons, New York.
9. T. Tang and P. Sheng (Eds), Nano Science and Technology – Novel Structures and Phenomena, Taylor & Francis, New York, 2004.
10. A. Nabok, Organic and Inorganic Nanostructures, Artech House, Boston, 2005.
11. J. M. Lehn, Supramolecular Chemistry – Concepts and Perspectives, V. C. H, 1995.

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