M.Sc.

CHEMISTRY

4th SEMESTER

SPRING 2019

CCS 504- ORGANIC CHEMISTRY SPECIALIZATION III [Credit-4](Elective Specialization)

UNIT I: **Organometallic Chemistry of Transitional Elements**

Preparative structural and characteristic aspects. Bonding of hydrocarbon ligands, metallocenes, oxidative insertion, reductive elimination, ligand migration from metal to carbon; organometallics as electrophiles. Davies rules, catalytic nucleophilic addition and substitution, coupling reactions, Heck, Suzuki and Stille reactions, hydrogenation hydroformylation, carbonylation of methanol, oxidations, alkene polymerisation, Ziegler-Natta reaction, olefin metathesis, Tebbe's reagent, Pauson-Khand reaction, Volhardt cotrimerisation. Fluctional organometallic compounds. Chemistry and use of organo-derivatives of non-transitional metals- tin, thalium, mercury, lead.

UNIT II: **Synthetic Methodology II**

Organophosphorus compounds-Chemistry of organophosphorus compounds, phosphorus ylids and chiral phosphines.

Organosulphur compounds-Chemistry of organo sulphur compounds, sulphur stabilized anions and cations, sulphonium salts, sulphonium and sulphoxonium ylids, chiral sulphoxide.

Organosilicon compounds - Synthetic uses of silyl ethers, silylenol ethers, TMSCl, TMSI, TMSCN, alkene synthesis, alkynyl, vinyl, aryl, allyl and acylsilanes; Brook rearrangement, silicon Baeyer Villiger rearrangement

UNIT III: **Advanced Pericyclic Reactions**

General perturbation molecular orbital theory in cycloadditions : Reactivity, regioselectivity and periselectivity. Cheletropic reactions, 1,3-dipolar cycloadditions, cycloaddition involving more than 6 electrons, charged species, three-component and four component cycloadditions. Ene reactions, group-transfer reactions and eliminations. Electrocyclic reactions of charged systems (cations and anions) Sigmatropic rearrangements : [1,j] shifts-[1,5] and [1,7] carbon shifts in neutral systems and [1,4] shifts in charged species : [i,j] shifts- [3,3] shifts, fluctional molecules; [5,5] shifts, [2,3] shifts in ylids.

CCS 506- ORGANIC CHEMISTRY SPECIALIZATION V (Credit-2)(Elective Specialization)

Oxidation and Reduction of Functional Groups

UNIT I: **Oxidation reactions:** Oxidation of hydrocarbons, oxidation of alcohols by various reagents, and methods, oxidation of carbon-carbon double bonds to diols and epoxides, Woodward and Prevost Reaction, synthetic reactions of epoxides, diastereo-selective

epoxidation of homoallylic alcohols, photosensetised oxidation of alkenes, oxidation of ketones to αβ- unsaturated ketones. Oxidation with ruthenium tetroxide, iodobenzene diacetate, and thallium (III) nitrate.

UNIT II: **Reduction reactions:** Catalytic hydrogenation-the catalyst, selectivity of reduction, reduction of functional groups,stereochemistry and mechanism, homogeneous hydrogenation. Reduction by dissolving metals-reduction with metal and acid, reduction of carbonyl compounds, Birch Reduction. Reduction by hydride transfer reagents-aluminium alkoxides, LAH and $NaBH_4$, lithiumhydridoalkoxyaluminates, lithiumaluminiumhydride aluminiumchloride reagents, diisobutylaluminiumhydride, sodiumcyanoborodydride, trialkylborohydrides. Other methods-desulphurisation of thio-acetals, di-imides, low-valent titanium species, trialkyltinhydrides.

CCS 507- ORGANIC CHEMISTRY SPECIALIZATION VI (Credit-2)(Elective Specialization)

Photo Organic Chemistry and Free Radical Reactions

UNIT I: **Photo Organic Chemistry:** Basic principles, Jablonsky diagram, exciplex, photochemistry of alkenes-intramolecular reactions of olefinic bond- geometrical isomerism, cyclization reactions, rearrangements of 1,4 and 1,5 dienes. Photochemistry of carbonyl compounds intramolecular reactions of saturated-, cyclic- and acyclic-, α,β-unsaturated- and γ,β-unsaturated carbonyl compounds, cyclohexadienones. Intramolecular cycloaddition reaction dimerization and oxetane formation. Norrish type I and type II reactions, di-pi-methane rearrangements. Photochemistry of aromatic compounds : isomerisation, addition and substitution reactions. Miscellaneous photochemical reactions. Photo-Fries reactions of anilides, Photo-Fries rearrangement, Barton reaction.

UNIT II: **Free Radical Reactions**: a) Methods of generation and detection of free radicals (trapping, ESR, NMR- CIDNP). b) Reactivity pattern of radicals, substitution and addition reactions, neighbouring group assistance. Reactivity of typical aromatic and aliphatic substractes at a bridge head, the effect of solvent on reactivity, oxidation of aldehydes to carboxylic acids, autooxidation, coupling of alkynes. Radical rearrangement. c) Radical cations and radical anions, single electron transfer reactions, SRN1 reactions.

CCS 515- INORGANIC CHEMISTRY SPECIALIZATION II (Credit-4)(Elective Specialization)

UNIT I: **NMR, ORD/CD**

NMR: ^{1}H,^{11}B,^{13}C,^{14}N,^{17}O,^{19}F and ^{31}P-NMR: instrumentation, chemical shift and application; fluxionality, distortion and dynamic equilibria; long-range spin-spin interaction; Identification of compounds like H_3PO_3, H_3PO_2, HPF_2, P_4S_3 etc. Adduct formation reaction: AsF_3 with SO_3. Exchange reaction – exchange in H_2O, factors affecting line width, evaluation of thermodynamic parameter with NMR, determination of reaction order, rate constant etc. from NMR. NMR spectra of paramagnetic ions. Contact shifts. Factors contributing to the magnitude of chemical shift. Applications involving the magnitude of coupling constant – $J_{^{13}C\text{-}H}$, $J_{Pt\text{-}P}$, $J_{P\text{-}F}$ etc. NMR spectra of $B_3H_8^-$, $HP_2O_5^{3-}$, $TiF_4.2B$ (B as donor molecule); consequences of nucleii with quadrupole moment in NMR. Double resonance technique. Introduction to pulse and FT NMR, time domain vs. frequency domain, FID, CW vs. FT NMR, rotating frame of reference, relaxation time measurements instrumentation.

CD/ORD: The symmetry origin of the optical activity of molecules, The phenomena of Optical Rotatory Dispersion (ORD) and Circular Dichroism (CD): principle, methodology and applications, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application;

UNIT II: **EPR, NQR, Mossbauer**

EPR: hyperfine splitting in various systems, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, nuclear quadrupole interactions. Applications.

NQR: Basic theory, effect of magnetic field in the spectra, relationship between 'q' and molecular structure. Structural information from NQR spectra, Applications.

Mössbauer:Gamma ray emission and absorption by nuclei, Mossbauer effect — conditions, nuclear recoil, Doppler effect, instrumentation, chemical shift examples, quadrupole effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, Use of Mössbauer spectra in chemical analysis, typical spectra of iron and tin compounds,

UNIT III: **I.R., Raman, Mass, PES, ESCA**

I.R., Raman: Origin, absorption of radiation by molecular vibrations in polyatomic molecules, effects giving rise to absorption bands, group vibration, limitation of the concept, FTIR, NDIR techniques. Raman Spectrometry: Theory, instrumentation, mechanism of Raman Effect, effect in solids, liquids and gases, Use of symmetry considerations to determine the number of active infra red and Raman lines, differences of IR and Raman spectra, Laser Raman spectra. Application.

EI, CI, FD, FAB-Mass, MALDI-TOF; isotropic effect, fragmentation patterns and application in structure elucidation; Photoelectron spectroscopy: Photo excitation and photo ionization, core level (XPS, ESCA) and valence level (UPS) Photoelectron spectroscopy, XPS and UPS experiment, chemical shift, detection of atoms in molecules and differention of same element in different environment from XPS, information about the nature of molecular

orbital from UPS of simple diatomic molecule e. g. N_2, O_2, CO, HCl etc. ESCA: Introduction to Electron Spectroscopy for Chemical Analysis (ESCA), Application to the analysis of inorganic samples.

CCS 518- INORGANIC CHEMISTRY SPECIALIZATION V (Credit-2)(Elective Specialization)

Chemistry of Complex Equilibria

UNIT I: Different pH-potentiometric, spectrophotometric, voltammetric tools and methods (sloperatio, mole-ratio and Job's method of continuous variation) of measuring stability constants of complexes, Bjerrum half n method, stability of mixed ligand complexes and calculations; determination of composition, evaluation of thermodynamic parameters, factors influencing the stability of complexes, equilibria in biomolecular systems.

UNIT II: Characteisation of stability of mononuclear, polynuclear and mixed –ligand complexes in solution, determination of composition and stability constants of complexes by pH metric, spectrophotometric and polarographic methods. Conditional stability constants and their importance in complexometric (EDTA) titrations and solvent extraction of metal ions. Statistical and nonstatistical factors influencing stability of complexes in solution, stability and reactivity of mixed ligand complexes. Soluility Equilibria – quantitativeness of precipitation (of metal hydroxides, sulphides and chelates)

CCS 520- INORGANIC CHEMISTRY SPECIALIZATION VII (Credit-2)(Elective Specialization)

UNIT I: **Chemical Application of Group Theory**

Importance of group theory in inorganic chemistry, splitting of orbital and free ion terms in crystal fields, quantitative relationship between Oh & Td splittings, construction of energy level in infinitely strong crystal field, the effect of distortion on d-energy levels, vibronic coupling and vibronic polarization, utilization of symmetry and group theory in constructing the MO diagrams of polyatomic molecules, coordination complexes including metallocene complexes. Symmetry of normal vibration, normal mode analysis, selection rules for IR and Raman transitions.

UNIT II: **Principle of symmetry in Chemistry**

Concept of symmetry in molecules, symmetry elements and symmetry operations, combining symmetry operations. Multiplication Table by stereographic projection technique. Elements of Group Theory, Sub groups and classes of group elements. Symmetry point groups of molecules, systematic classification of molecular point groups, Application of symmetry in identifying polar and chiral molecules; Symmetry and stereo-isomerism. Unit vector transformation and interpretation of character table. Identification of symmetry label of MO

in a molecule. Construction of MO on the basis of Symmetry of the molecules (H_2O, NH_3, B_2H_6, CH_4). Two dimensional space group.

CCS 527- PHYSICAL CHEMISTRY SPECIALIZATION II (Credit-4)(Elective Specializaition)

UNIT I: **Group Theory-Introduction**

Symmetry Elements and Point Group: Symmetry in nature, symmetry elements and symmetry operations. Symmetry properties of atomic orbitals. Elements of group theory. Elements of group theory: groups, subgroups, classes and characters, classes of symmetry operations, symmetry point groups; representation of groups by matrices. Representation of symmetry operator transformation of basis vector, Symmetry transformation of operators; The Great Orthogonality Theorem (without proof) and its consequences; construction and applications of character tables, representation of cyclic groups. direct product and projection operator and their applications; symmetry adapted linear combination (SALC)s.

UNIT II: **Photochemistry**

Jablonski diagram, Fluorescence and phosphorescence, Delayed fluorescence, quantum yield, Mechanism and decay kinetics of photophysical processes. Fluorescence quenching (dynamic and static), Stern - Volmer equation. Energy transfer (Forster's dipole coupling), Electron Transfer phenomenon (Marcus theory, Rehm Weller theory), Proton transfer phenomenon, complex formation phenomenon (excimer, exciplex). Interaction of electromagnetic radiation with matter, Transition probabilities, Transition moment integral and its applications. Electric and megnetic dipole moments. Selection rules. Violation of Franck Condon principle, oscillator strength. Nature of transitions (e.g., n–π*, π–π*, d–d, charge transfer) solvent effect on absorption and emission spectra, Stoke's shift. Properties of electronically excited molecules: Life–time, redox potential, dipole moment, pK values. Potential energy diagram for donor acceptor system, Polarized luminescence. Nonradiative intramolecular electronic transition; internal conversion, inter-system crossing. Crossing of potential energy surface (Franck-Condon factor). Adiabatic and non adiabatic cross over. Kasha's rule.

UNIT III: **Electrochemistry**

Ion Solvent interactions: Concept, experimental determination, application to equilibria, kinetics, universal scales of potential acidity and basicity in different solvents. Born Model & Eley-Evans model, Absolute heats of hydration (Halliwel & Nyburg Method). Solvation number and its determination. Ion-solvent-non-electrolyte interactions: Salting-in and salting-out phenomena. Structure of electrified interfaces, electrical double layers and 'zeta potential'.

Ion-Association: Bjerrum and Fuoss equation for ion-pair formation. Conductance minima, Ion- triplet, Ion-quadruplets; Walden's empirical rule and Fuoss treatment of conductance minima. Fuoss Shedlovsky's method of determination of association constant.

Ion-transport in solution: Limiting Debye Huckel-Onsager Expression. (Electrophoretic effect, Relaxation effect and time of relaxation). Transport number as a function of concentration. Wien Effect, Debye-Falkenhagen effect, Nernst Hartley Expression, Viscosity B-Coefficients.

Rate equation for electrode processes; Kinetic derivation of the Nernst equation. Overvoltage. Butler-Volmer equation, Tafel equation, exchange current density. electrolytic conductance – Kohlrausch's law and its applications. Phenomenon of corrosion- electrochemical view.

CCS 530- PHYSICAL CHEMISTRY SPECIALIZATION V (Credit-2)(Elective Specialization)

Principles & Basic Instrumentation of NMR/ESR/NQR/Mossbauer Spectra

UNIT I: *Nuclear Magnetic Resonance (NMR) Spectroscopy*: Basic instrumentation, nuclear spin, nuclear resonance, saturation, shielding of magnetic nuclei, chemical shift, and its measurements, factors influencing chemical sift, deshielding, spin-spin interactions, factors influencing coupling constant `J`. Classification of molecules: (ABX, AMX, ABC, A_2B_2, etc. types), spin decoupling. FT NMR (qualitative idea) and its advantages, Applications of NMR in medical diagnosis.

UNIT II: *Electron Spin Resonance (ESR) Spectroscopy*: Basic principles, zero field splitting, and Kramer`s degeneracy, factors affecting the `g` value. Isotropic and anisotropic hyperfine coupling constants, spin Hamiltonian, spin densities and McConnell relationship.

UNIT IIII: *Nuclear Quadruple Resonance (NQR) Spectroscopy*: Qudrupole nuclei, qudrupole moments, electric field gradient, coupling constant, splitting and simple applications.

UNIT IV: *Mössbauer (MB) Spectroscopy*: Basic principle, instrumentation, spectral parameters and spectrum display, center shift, qudrupole and magnetic interactions.

CCS 531- PHYSICAL CHEMISTRY SPECIALIZATION VI (Credit-2)(Elective Specialization)

Applications of NMR/ESR/Mossbauer Spectra

UNIT I: *NMR phenomenon*, spin ½ nuclei, (^{1}H, ^{13}C, ^{31}P and ^{19}F), ^{1}H NMR, Zeeman splitting, effect of magnetic field strength on sensitivity and resolution, chemical shift d, inductive and anisotropic effects on d, chemical structure correlations of d, chemical and magnetic

equivalence of spins, spin-spin coupling, structural correlation to coupling constant J, first order patterns. Multinuclear NMR of B, Al, Si, F and P nuclei; structure and dynamics of representative inorganic molecules, deriving activation and thermodynamic parameters;

UNIT II: Introduction to 2D NMR: NOESY, COSY, HETCOR, HOMCOR, INADEQUATE, INDOR, INEPT for simple compounds and problems.

UNIT III: *ESR*: hyperfine splitting in various systems, factors affecting the magnitude of g-value, Anisotropy in the hyperfine coupling constants, zero-field splitting and Kramers' degeneracy, nuclear quadrupole interactions, Application.

UNIT IV: *Mössbauer*: Gamma ray emission and absorption by nuclei, Mössbauer effect, Isomer shift, quadrupole splitting, Application to the elucidation of structure and bonding of Fe^{III} and Fe^{II}, Sn^{IV} and Sn^{II} compounds, detection of oxidation states and inequivalent MB atoms.

CCS 541- COMPUTER APPLICATIONS IN CHEMISTRY-I - (Credit-4)(Core Open)

Introduction to programming languages; basic numerical analysis: solution of nonlinear equations using Newton-Raphson method (e.g. finding the roots of a cubic equation – vander Waals equation), solution of linear systems using Gaussian elimination, interpolation, numerical integration (trapezoidal and Simpson's 1/3rd rule), numerical solution of differential equations (Euler and Runge-Kutta method). Fourier transformations and applications in spectroscopy. Use of molecular geometry optimisation software (Gaussian 09); construction of z-matrix and concept of force field. Classical Molecular Dynamics (MD) simulation and application to simple systems like Lennard-Jones fluids. [Effort should be made to reproduce data reported in the literature using the above mentioned numerical methods wherever possible.]

CCS 565 M.Sc. Project (Core Compulsory) Credit 4(Core Compulsory)

CCS 564 ASSYMETRIC ORGANIC SYNTHESIS/CATALYSIS Credit 2

Inorganic Chemistry Books

1. Advanced Inorganic Chemistry- F. A. Cotton & G. Wilkinson, John Wiley

2. Inorganic Chemistry- J.E. Huheey, E.A. Keiter & R. L. Keiter, Harper & Row

3. Chemistry of Elements- N. N. Greenwood & A. Earnshaw

4. Concept and Models of Inorganic Chemistry-Douglass, McDaniel & Alexander

5. Coordination Chemistry- S. F. A. Kettle

6. Theoretical Approach to Inorganic Chemistry-A. F. Willams

7. Inorganic Chemistry-D. F. Shriver, P. W. Atkins & C. H. Langford

8. Chemical Applications of Group theory- F. A. Cotton

9. Molecular Symmetry & Group Theory- R. L. Carter

10. Introduction to Ligand Fields- B. N. Figgis

11. Introduction to Ligand Field Theory- C. J. Ballahausen

12. Valence- C. A. Coulson

13. Chemical Crystallography-L. W. Bunn

14. Solid State Chemistry- C. N. R. Rao

15. Ionic Crystal Lattice & Nonstoichiometry-N. N. Greenwood

16. Inorganic Reaction Mechanism- M. L. Tobe

17. Mechanism of Inorganic Reactions- Katakis & Gordon

18. Kinetics and Mechanism of Reactions of Trans. Metal Complexes- R. G. Wilkins

19. Determination and use of Stability Constants- A. E. Martell & R. J. Motekaitis

20. An Introduction to Bioinorganic Chemistry-D. R. Williams

21. Inorganic Chemistry of Biological Processes-M. N. Hughes

22. Bioinorganic Chemistry-E. I. Ochiai

23. Bioinorganic Chemistry- R. W. Hay

24. Elements of Bioinorganic Chemistry- G. N. Mukherjee & A. Das

25. Organometallic Chemistry of Transition Metals-R.H. Cabtree

26. Organometallic Chemistry- R. C. Mehrotra & A. Singh

27. Nuclear and Radio Chemistry-Friedlander, Kennedy & Miller

28. Radioactiviry Applied to Chemistry- A. C. Wahl & N. A. Bonner

29. Magnetochemistry- Selwood

30. Intriduction to Magnetochemistry- Earnshaw

31. Environmental Analysis- S. M. Khopkar

32. Physical Methods in Inorganic Chemistry-R. S. Drago

33. Instrumental Methods in Chemical Analysis- Willard, Meritt and Dean

34. Instrumental Methods in Chemical Analysis- G. W. Ewing

35. Vogel`s Text Book of Quantitative Chemical Analysis G. H. Jeffery, J. Bassett, J. Mendham & R. C. Denny

36. Advanced Experiments in Inorganic Chemistry-G. N. Mukherjee (U. N. Dhur)

37. Macro and Semi-micro Qualitative Inorganic Analysis- A. I. Vogel

38. Semi-Micro Qualitative Inorganic Analysis- G. N. Mukherjee (C.U.Press)

39. Quantitative Chemical Analysis- Kolthoff, Sandel, Meehan & Bruckenstein

40. Synthesis and Characterizations of inorganic Compounds-W. L. Jolly

41. Group Theory – Bishop (D.M.)

42. Electron Transfer reaction: ISM & OSM – Purcell & Kotz

Organic Chemistry Books

1. Organic Chemistry- I. L. Finar, Vols. 1 & 2, ELBS

2. .Adv. Organic Chemistry: Reaction, Mechanism- Jerry March

3. Adv. Organic Chemistry-F. A. Carey & R. J. Sundberg

4. Organic Chemistry (3rd. edn) -Hendrikson, Cram, Hammond

5. Organic Chemistry- Clayden, Greeves, Warren & Wolthers

6. Organic Chemistry- R. T. Morrison & R. N. Boyd

7. Organic Reaction Mechanics- A. Gallego, M. Gomer & M. A. Sierra

8. A Guide Book to Mechanism of Organic Reactions-Peter Sykes

9. Reaction Mechanism in Organic Chemistry- S. M. Mukherjee & S. P. Singh

10. Structure and Mechanism in Organic Chemistry- C. K. Ingold

11. Physical Organic Chemistry-J. Hiine

12. Physical Organic Chemistry-N. S. Isaacs

13. Orbital Symmetry and Organic Reactions-T. L. Gilchrist & R. C. Storr

14. Some Modern Methods in Organic Synthesis-W. Carruthers

15. Principles of Organic Synthesis-Norman, Coxon & Blakie

16. Current Trends in Organic Synthesis-C.Scolastico & F. Nicotra

17. Frontier Orbitals and Organic Chemcal Reactions-I. Fleming

18. Pericyclic Reactions- Gill & Willis

19. Pericyclic Reactions- S. M. Mukherjee

20. Stereochemistry-E. Eliel & S. H. Wilen

21. Stereochemistry- D. Nasipuri

21a. Stereochemistry of Organic Compounds- P. Kalsi

22. NMR in Chemistry-A Multinuclear approach—W. Kemp

23. Application of N. M. R. Spectroscopy in Organic ChemistryL- L. M. Jackman M.

24. Interpretation of ^{13}C –NMR Spectra- F. W. Werli & T. W. Wirthlin

25. Mass Spectrometry-Organic Applications-K. Biieman

26. Free Radicals in Organic Chemisrey—Fossey, Lepost & Sorbs

27. Elements of Organic Photochemistry-D. O. Cowan & K. L.Drisco

28. Application of Organotransition Metal in Organic Synthesis-S.G. Davies

29. Comprehensive Heterocyclic Chemistry- A. R. Katritzky, & C. W. Rees (eds)

30. Heterocyclic Chemistry-J. A. Joule &K. Mills

31. Natural Product-A. Pelter

32. Natural Products: Chemistry & Biological Significance Mann, Davidson, Hobbs, Banthrope, Harbome & Longman

33. An Introduction to Medicinal Chemistry-(3rd.edn) G. L. Patrick

34. Fundamentals of Medicinal Chemistry-G. Thomas

35. Supramolecular Chemistry: Concepts & Perspective- J. M. Lehn

36. Experimental Organic Chemistry: Principles & Practice-L. M. Harwood & C. J. Roodey

37. Experiments and Techniques in organic Chemistry-Pasto, Johnson & Miller

38. Spectrometric Identification of Organic Compounds-(6th. edn)-Silverstein & Webster

39. An Introduction to Experimental Organic Chemistry- Robert, Gilbert, Rodewaid & Wingrove

40. Systematic Qualitative Organic Analysis-H. Middleton

41. Hand Book of Organic Analysis- H. T. Clarke 42. Text Book of Practical Organic Chemistry-A.I. Vogel

42. Aromaticity and Aromatic Character – G.M. Badger

Physical Chemistry Books

1. Physical Chemistry: A Molecular Approach-D. A. McQuarrie & J. D. Simon

2. Physical Chemistry- R. S. Berry, S. A. Rice & J. Ross

3. Introduction to Quantum mechanics- L. Pauling & E. B. Wilson

4. Quantum Mechanics J. L. Powel & B. Crasemann

5. Elementary Quantum Chemistry-F. L. Pilar

6. Quantum Chemistry- I. N. Levine

7. Chemical Kinetics-K. J. Laidler

8. Fundamentals of Chemical Kinetics-S. W. Benson

9. Theoretical Chemistry- S. Glasstone

10. The Principles of Chemical Equilibrium-K. Denbigh

11. The Physical Chemistry of Surfaces- N. K. Adams

12. Physical Chemistry of Surfaces- A. W. Adamson

13. Introduction to Molecular Spectroscopy-G. M. Barrow

14. Fundamentals of Molecular Spectroscopy- C.W. Banwell

15. Introduction to Quantum Mechanics- D. J. Griffith

16. Group Theory and Chemistry—D. M. Bishop

17. Thermodynamics and an Introduction to Thermostatistics- H. B. Callen

18. Coulson`s Valence- R. McWeeny

19. Modern Electrochemistry-J.O`M. Bockris & A. K. N. Reddy

20. Principles of Physical Biochemistry- K. E. van Holde, C. Johnson & P. S. Ho

21. Polymer chemistry-P. J. Flory

22. Microwave Spectroscopy-C. H. Townes & A. L. Schawlow

23. Symmetry and Spectroscopy- D. C. Harris & M. d. Bertolucci

24. Solid State Physics- A. J. Dekker

25. Introduction to Solid State Physics- C. Kittel

26. Chemical Kinetics and Dynamics- J. I. Seinfeld, J. S. Francesco & W. L. Hase

27. Text Book of Physical Chemistry- S. Glasstone

28. Statistical Mechanics- D. A. Mcquarrie

29. Statistical Mechanics-B. B. Laud

30. Statistical Mechanics- K. Huang

31. Practical Physical Chemistry- A. M. James & F. F. Prichard

32. Findlay's Practical Physical Chemistry- B. P. Levit

33. Experimental Physical Chemistry- Shoemaker & Garland

34. Introduction to Magnetic Resonance-A. Carrington & A. D. McLachlan

35. NMR, NQR, EPR and Mossbauer Spectro. in Inorganic Chemistry- R. V. Parish

36. Macromolecules:Structure and Function- F. Wold, Prentice-Hall

37. Principles of Biochemistry- A.L. Lehninger

38. Programming with FORTRAN - S. Lepschutz & A. Poe (Schaum Series)

39. Computer Programming in FORTRAN 77- V. Rajaraman

40. Computational Chemistry- A. C. Norris, John Wiley

41. Computational Chemistry- A. Konar

42. Computers in Chemistry – K. V. Raman, TMH

43. Electricity and Magnetism (Vol I) – J.H. Fewkes & J. Yarwood, OUP

44. Atomic Physics (Vol II) – J. Yarwood , OUP 45. Biochemistry – Voet and Voet

45. Kinetic and Mehanism – Frost &

46. Statistical Mechanics – T.H. Hill

Computer applications in chemistry

Suggested Readings

1. Rajaraman V., Computer Progoramming in FORTRAN 90 and 95, 4th edition, Pubs:Prentice Hall, India (2004).

2. Scheid F., Numerical Analysis: Schaum's Series, Pubs: McGraw Hill, Singapore (1988)