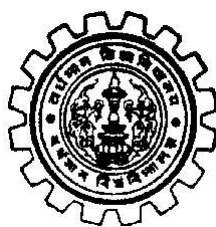


DRAFT SYLLABUS

M. Sc. Course in Chemistry

To be effective from the session 2020-21



THE UNIVERSITY OF BURDWAN

BURDWAN 713 104

WEST BENGAL, INDIA

www.buruniv.ac.in

Semester I

Course				Lecture Hour /week	Duration of Exam (Hour)	Marks			Credit
Course code	Type	T/ P	Name			I.A.	E.T	Total	
MSCH101	Core	T	Inorganic Gen-I	4H	2H	10	40	50	4
MSCH102	Core	T	Nuclear Analytical Gen-I	4H	2H	10	40	50	4
MSCH103	Core	T	Organic Gen-I	4H	2H	10	40	50	4
MSCH104	Core	T	Physical Gen-I	4H	2H	10	40	50	4
MSCH105	Core	P	Inorganic Practical	8H	4H	10	40	50	4
MSCH106	Core	P	Nuclear Analytical Practical	8H	4H	10	40	50	4
					Total credit				24

Semester II

Course				Lecture Hour /week	Duration of Exam (Hour)	Marks			Credit
Course code	Type	T/P	Name			I.A.	E.T	Total	
MSCH201	Core	T	Inorganic Gen-II	4H	2H	10	40	50	4
MSCH202	Core	T	Nuclear Analytical Gen-II	4H	2H	10	40	50	4
MSCH203	Core	T	Organic Gen-II	4H	2H	10	40	50	4
MSCH204	Core	T	Physical Gen-II	4H	2H	10	40	50	4
MSCH205	Core	P	Organic Practical	8H	4H	10	40	50	4
MSCH206	Core	P	Physical Practical	8H	4H	10	40	50	4
					Total credit				24

Semester III

Course				Lecture Hour /week	Duration of Exam (Hour)	Marks			Credit
Course code	Type	T/ P	Name			I.A.	E.T	Total	
MSCH301	Core	T	Inorganic Advance General	4H	2H	10	40	50	4
MSCH302	Core	T	Nuclear Analytical Advance General	4H	2H	10	40	50	4
MSCH303	Core	T	Organic Advance General	4H	2H	10	40	50	4
MSCH304-M*	GE	T	Basics in Medicinal Chemistry	2H	1H	05	20	25	2
MSCH304-I*	GE	T	Basics in Industrial Chemistry	2H	1H				
MSCH305-I	DE	T	Inorganic Major-I	4H	2H	10	40	50	4
MSCH305-N	DE	T	Nuclear Analytical Major-I	4H	2H				
MSCH305-O	DE	T	Organic Major-I	4H	2H				
MSCH305-P	DE	T	Physical Major-I	4H	2H				
MSCH306-I	DE	P	Inorganic Major-I Practical	8H	4H	10	40	50	4
MSCH306-N	DE	P	Nuclear Analytical Major-I Practical	8H	4H				
MSCH306-O	DE	P	Organic Major-I Practical	8H	4H				
MSCH306-P	DE	P	Physical Major-I Practical	8H	4H				
MSCH307	**	N. A.	Social Outreach	N.A.	N.A.	5	20	25	2
					Total credit				24

*Minor elective

Semester IV

Course				Lect. Hour / week	Duration of Exam (Hour)	Marks			Credit
Course code	Type	T/P	Name			I.A	E.T	Total	
MSCH401	Core	T	Physical Advance General	4 H	2 H	10	40	50	4
MSCH402	Core	T	Medicinal Chemistry	4 H	2 H	10	40	50	4
MSCH403-I	Floating	T	Inorganic Major-II	4 H	2 H	10	40	50	4
MSCH403-N	Floating	T	Nuclear Analytical Major-II	4 H	2 H				
MSCH403-O	Floating	T	Organic Major-II	4 H	2 H				
MSCH403-P	Floating	T	Physical Major-II	4 H	2 H				
MSCH404-I	DE	T	Inorganic Major-III	4 H	2 H				
MSCH404-N	DE	T	Nuclear Analytical Major-III	4 H	2 H	10	40	50	4
MSCH404-O	DE	T	Organic Major-III	4 H	2 H				
MSCH404-P	DE	T	Physical Major-III	4 H	2 H				
MSCH405-I	DE	P	Inorganic Major-II Practical	8 H	4 H				
MSCH405-N	DE	P	Nuclear Analytical Major-II Practical	8 H	4 H	10	40	50	4
MSCH405-O	DE	P	Organic Major-II Practical	8 H	4 H				
MSCH405-P	DE	P	Physical Major-II Practical	8 H	4 H				
MSCH406-I	Project/ Term paper	N.A	Inorganic	4H	---				
MSCH406-N	Project/ Term paper	N.A	Nuclear Analytical	4H	---	---			
MSCH406-O	Project/ Term paper	N.A	Organic	4H	---	---			
MSCH406-P	Project/ Term paper	N.A	Physical	4H	---	---			
					Total credit				24

Semester-I (Total Marks 300, Credit: 24)

Core Subject

MSCH101: Inorganic General-I

Marks: 50, Credit: 4

1. Bonding and properties in chemical systems – a quantum chemical approach

The Born-Oppenheimer approximation, Molecular Orbital Theory (MOT), Linear Combination of Atomic Orbitals (LCAO), LCAO-MO method, MO of homo- and heteronuclear diatomic molecules, MO of polynuclear AB_n type molecules, Walsh diagram: Prediction of geometry of AB_2 type molecules, Molecular term symbols, Huckel method of π -MO calculation in ethylene, allyl system, etc, Frost diagram of carbocyclic π -systems

2. Coordination chemistry – stereochemistry, bonding, geometric and electronic structures

Fundamentals, Orgel diagram, Tanabe-Sugano diagram, ligand symmetry orbital, molecular orbital, spectral properties, Nephelauxetic effect, Racah parameter, vibronic coupling, band broadening, spin-orbit coupling, spin-forbidden transition, intensity stealing, magnetic properties, anomalous and subnormal magnetic moments, lowering of symmetry, electronic, steric, Jahn-Teller and Renner-Teller effects on energy levels, conformation of chelator/congregator, structural equilibrium and implication, Correlation of CFSE with spectroscopy

3. Organometallic chemistry I

Overview and striking difference, valence electron count, oxidation number and formal ligand charge; carbonyl ligand, pi-ligands: linear pi systems and cyclic pi systems, complexes containing M-C, M=C and M \equiv C bonds, hydride and dihydrogen complexes, phosphines and related ligands, spectral analysis and characterization, Dewar-Chatt-Duncanson bonding model, isolobal analogy, Agostic interaction

4. Emulsion chemistry

Introduction, industrial applications, the interface, thermodynamics of emulsion formation and breakdown, van der Waals attraction, electrostatic repulsion, steric repulsion, Gibbs adsorption isotherm, mechanism of emulsification, method of emulsification, role of surfactants in emulsion formation, role of surfactant in droplet deformation, Hydrophilic-Lipophilic Balance (HLB) concept, phase inversion temperature (PIT) concept, Cohesive Energy Ratio (CER) concept, critical packing parameter for emulsion selection, creaming, sedimentation, flocculation, Ostwald ripening, coalescence, phase inversion, rheology

Recommended Books

- H. E. White, *Introduction to Atomic Spectra*, McGraw-Hill Kogakusha Ltd, Tokyo, 1934.
- B. N. Figgis, *Introduction to Ligand Field Theory*, Interscience, New York, 1966.
- C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.
- R. McWeeney, *Coulsons' Valence*, 3rd Edn, Oxford University Press, Oxford, 1979.
- A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.
- B. E. Douglas and C. A. Hollingsworth, *Symmetry in Bonding and Spectra, An Introduction*, Academic Press, New York, 1985.
- T. A. Albright, J. K. Burdett and M. H. Whangbo, *Orbital Interactions in Chemistry*, Wiley, New York, 1985.
- V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.
- K. Fukui and H. Fujimoto, *Frontier Orbital and Reaction Paths*, World Scientific, Singapore, 1995.
- J. G. Verkade, *A Pictorial Approach to Molecular Bonding*, 2nd Edn, Springer-Verlag, New York, 1997. A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.
- F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley & Sons, Inc, New York, 1999.
- B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley & Sons, Inc., New York, 2001.
- G. Wulfsberg, *Inorganic Chemistry*, Viva Books Pvt Ltd, New Delhi, 2001.
- J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Edn, Pearson, New Delhi, 2006.
- D. A. McQuarrie, P. A. Rock and E. B. Gallogly, *General Chemistry*, 4th Edn, University Science Books, Mill Valley, Canada, 2011.
- A. K. Mukherjee, B. C. Ghosh, *Group theory in Chemistry: Bonding and molecular spectroscopy*, Universities press, 2018
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.
- J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.
- D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University Press, 2001.
- M. Cox, *Optical Properties of Solids*, Oxford University Press, Oxford, 2001.
- G. Aruldas, *Molecular Structure and Spectroscopy*, 2nd Edn, Prentice-Hall of India, New Delhi, 2007.
- C. Trindle and D. Shillady, *Electronic Structure Modeling: Connection between Theory and Software*, CRC Press, Boca Raton, FL, 2008.
- P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry*, 4th Edn, Oxford, 2006.

- I. Pelant and J. Valenta, *Luminescence Spectroscopy of Semiconductors*, Oxford, New York, 2012.
- O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
- G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.
- C. N. Satterfield, *Heterogeneous Catalysis in Practice*, McGraw-Hill, New York, 1980.
- P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn, Chapman and Hall, London, 1988.
- J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, VCH, New York, 1997.
- R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 4th Edn, Wiley, New York, 2005.
- C. Elschenbroich, *Organometallics*, 3rd Edn, Wiley-VCH, Weinheim, 2006.
- R. A. van Santen and M. Neurock *Molecular Heterogeneous Catalysis*, Wiley-VCH, Weinheim, 2006.
- G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, International 2nd Edn, Oxford University Press, Oxford, 2010.
- J. F. Hartwig, *Organotransition Metal Chemistry. From Bonding to Catalysis*, University Science Books, Sausalito, CA, 2010.
- S. J. Lippard and J. M. Berg, *Principles of Bioinorganic Chemistry*, University Science Books, Mill Valley, CA, 1993.
- W. Kaim and B. Schwederski, *Bioinorganic Chemistry: Inorganic Elements in the Chemistry of Life*, Wiley, New York, 1994.
- I. Bertini, H. B. Gray, S. J. Lippard and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi, 1998.
- A. Das and G. N. Mukherjee, *Elements of Bioinorganic Chemistry*, 2nd Edn, U. N. Dhur and Sons, Kolkata, 2002.
- A. K. Das, *Bioinorganic Chemistry*, Books & Allied (P) Ltd. Kolkata 2007.
- E. Ochiai, *Bioinorganic Chemistry: A Survey*, Academic Press, Elsevier, 2009.
- R. R. Crichton, *Biological Inorganic Chemistry: A New Introduction to Molecular Structure*, 2nd Edn, Elsevier, New York, 2012.
- R. M. Roat-Malone, *Bioinorganic Chemistry: A short Course*, 2nd Edn, Wiley, New York, 2013.
- G. Patrick, *Instant Notes: Medicinal Chemistry*, Viva Books, New Delhi, 2002.
- G. L. Patrik, *An Introduction to Medicinal Chemistry*, 3rd Edn, Oxford University Press, 2006.
- A. Kar, *Medicinal Chemistry*, 4th Edn, New Age International (P) Ltd, New Delhi, 2007.
- C. G. Wermuth (Ed), *The Practice of Medicinal Chemistry*, Academic Press, Noida, India, 2008.
- D. Sriram and P. Yogeewari, 2/e, *Medicinal Chemistry*, Pearson
- G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3/e, Pearson.
- A. G. Sharpe, *Inorganic Chemistry*, 3/e, Pearson
- A. F. Hill, *Organotransition Metal Chemistry*, Royal Society of Chemistry, London, 2002.

MSCH102: Nuclear-Analytical General I**Marks: 50, Credit: 4**

1. Nuclear properties and structure I

Fundamentals, nuclear angular momentum, magnetic dipole moment and electronic quadrupole moment, parity of nuclear energy states; nuclear size and root mean square radius of atomic nucleus

2. Radioactive equilibrium

Successive disintegration, Bateman equation, secular and transient equilibrium, no equilibrium; analysis of special types of successive disintegration, formation of radioelement in a nuclear reaction, activation analysis (introductory)

3. Interaction of radiation with matter

Different radiations, interactions of heavy charged particles, charged particles and photons, energy loss, stopping power and related semi-empirical calculations, Bethe formula, collisional and radiative stopping power, mean excitation energy, range, slowing down time, Cerenkov radiation, attenuation coefficient

4. Statistical methods in analytical chemistry

Application of counting statistics in analytical and nuclear measurements: probability and binomial distribution, radioactivity as a statistical phenomenon, standard deviation of counting data, Poisson distribution, optimization of counting experiments

5. Thermal methods

Different methods of analysis: thermogram, TGA, DTA, DSC, applications, thermo-chemiluminescence, different types of titrations and their applications,

6. Environmental chemistry

Hazardous and Radioactive wastes, Treatment, waste management, volatile organic compounds, corrosion and protection of metals, pollution control in Paper and pulp industries, Petroleum refineries and petrochemical units, Fertiliser industries, Tanning, Sugar, Alcohol, Electroplating & metal finishing etc.

Recommended Books

- B. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice Hall, New York, 1965.
- S. Glasstone, *Source Book of Atomic Energy*, East-West Press Private Ltd, New Delhi, 1967.
- R. D. Evans, *The Atomic Nucleus*, McGraw-Hill, New York, 1979.
- G. R. Choppin and J. Rydberg, *Nuclear Chemistry: Theory and Applications*, Pergamon Press, Oxford, 1980.
- G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, *Nuclear and Radiochemistry*, 3rd Edn, Jhon Wiley & Sons Inc, New York, 1981.
- H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4th Edn, New Age International (P) Ltd Publications, New Delhi, 2001.
- D. D. Sood, A.V. R Reddy and N. Ramamoorthy, *Fundamentals of Radiochemistry*, Yancas, Mumbai, 2004.
- W. D. Loveland, D. J. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, Wiley Interscience, New Jersey, 2006.
- C. Duval, *Inorganic Thermogravimetric Analysis*, Elsevier Publishing Co, New York, 1963.
- W. W. Wendlandt, *Thermal Methods of Analysis*, Interscience Publishers, New York, 1964.
- R. C. McKenzie (Ed), *Differential Thermal Analysis*, Academic Press, New York, 1970.
- D. Dollimore, *General Review on Thermal Analyses*, Anal Chem, 1994, 66, 17R.
- P. Tundo, A. V Perosa and F Zecchimi (Eds), *Methods and Reagents for Green Chemistry: An Introduction*, Wiley Interscience, New Jersey, 2007.
- R. K. Sharma, I. T. Sidhwami and M. K. Chaudhury, *Green Chemistry experiments: A Monograph*, Tucker Prakashan, New Delhi, 2007.
- R.Sanghi and M. M. Srivastava, *Green Chemistry, Environment Friendly Alternatives*, Narosa, New Delhi, 2008.
- R.Sanghi and V. Singh, *Green Chemistry for environmental remediation*, Wiley, New York, 2012.
- J. H. Seinfeld, *Air Pollution: Physical and Chemical Fundamentals*, McGraw-Hill, New York, 1975.
- O. Hutzinger (Ed), *The Handbook of Environmental Chemistry*, Springer-Verlag, Weinheim, 1980.
- D. F. S. Natusch and P. K. Hopke, *Analytical Aspects of Environmental Chemistry*, John Wiley & Sons, New York, 1983.
- R. M. Harrison (Ed), *Pollution: Causes, Effects and Control*, Royal Society of Chemistry, Great Britain, 1990.
- J. E. Fergusson, *The Heavy Elements: Chemistry, Environmental Impact and Health Effects*, Pergamon Press, Oxford, 1990.
- S. E. Manahan, *Environmental Chemistry*, Lewis Publishers, Boston, 1991.
- A. K. De, *Environmental Chemistry*, 4th Edn, New Age International (P) Ltd Publications, New Delhi, 2000.
- Arabinda Kumar Das, "Elements of Green Chemistry with Green Laboratory Experiments, Readers Service, Kolkata

MSCH103: Organic General I**Marks: 50, Credit: 4****1. Conformation and reactivity of cyclic systems**

Introduction, reactions on small rings (four and five membered rings), Stereochemical control in six-membered rings: stereoselectivity in reactions, conformational control in ring formation; Stereoselective reactions of bicyclic compounds: bridged, fused and spiro

2 Structure-reactivity relationship

A quantitative approach to Linear free energy relations: Hammett equation, Hammett's σ_x and ρ values and their physical significance, through conjugation; deviations from straight line plots; steric effects: Taft equation; solvent effects: Grunwald-Winstein equation

3 Heterocycles

Synthesis, reactivity and uses of imidazole, pyrazole, oxazole, isooxazole, thiazole, isothiazole, triazole and their derivatives

4 Proteins

Classification, evaluation quality: biological value, digestibility co-efficient, PER and NPU; denaturation, structure elucidation; amino acid analysis, molecular weight determinations, tertiary and quaternary structures

5 Polymers : Principles and synthesis

Monomer, dimer, dendrimer and polymer; mechanism of formation: carbonyl substitution reactions, electrophilic aromatic substitution, the SN^2 reaction and nucleophilic attack on isocyanates; polymerization of alkenes; co-polymerization; biodegradable polymers and plastics; reactions on polymers

6 Green Chemistry I

Principles and implementations; traditional and green synthesis of ibuprofen, adipic acid and maleic anhydride; use of green reagents, catalysts and solvents towards organic syntheses

Recommended Books

D. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn, Wiley Eastern, New Delhi, 1993.

E. L. Eliel, S.H. Wilen and L.N. Mander, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994.

R. S. Ward, *Selectivity in Organic Synthesis*, John Wiley & Sons, New York, 1999.

- F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry Part A and Part B*, 4th Edn, Plenum Press, New York, 2001.
- J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University Press, Oxford, 2001.
- J. R. Hanson, *Organic Synthetic Methods*, Royal Society of Chemistry, London, 2002.
- J. H. Fuhrhop and G. Li, *Organic Synthesis*, Concepts and Methods, Wiley-VCH, New York, 2003.
- P. Sykes, *A Guidebook to Mechanism in Organic Chemistry*, 6th Edn, Pearson Education Ltd, New Delhi, 2011.
- R. Karritzky, *Handbook of Heterocyclic Chemistry*, Pergamon Press, London, 1986.
- R. R. Gupta, M. Kumar, V. Gupta, *Heterocyclic Chemistry II*, Springer Pvt Ltd, India, 2005.
- R. K. Bansal, *Heterocyclic Chemistry*, 4th Edn, New Age International (P) Ltd, India, 2005.
- J. A. Joule, K. Mills, *Heterocyclic Chemistry*, 5th Edn, John Wiley & Sons Ltd, UK, 2010.
- K. Nakanishi, T. Goto, S. Ito, S. Natori and S. Nozoe, *Natural Products Chemistry*, Vol I, Academic Press, New York, 1974.
- M. P. Stevens, *Polymer Chemistry: An Introduction*, 3rd Edn, Oxford University Press, USA, 1998.
- G. R. Newkome, C. N. Moorefield and F. Vogtle, *Dendrimers and Dendron: Concepts, Syntheses, Applications*, Wiley-VCH, Weinheim, 2001.
- G. Odian, *Principles of Polymerization*, 4th Edn, Wiley Interscience, New Jersey, 2004.
- P. C. Hiemenz and T. P. Lodge, *Polymer Chemistry*, 2nd Edn, CRC Press, Boca Raton, FL, 2007.

MSCH104: Physical General I

Marks: 50, Credit: 4

1. Symmetry and group theory I

Point symmetry operations, groups and group multiplication tables, similarity transformation and conjugate classes, identification of point groups and stereographic projection, representation of symmetry operators and groups; characters of symmetry operators in a representation, invariance of character under similarity transformation, rules (without derivation) for construction of character tables with illustrations, symmetry elements and symmetry operations of the Platonic solids, symmetry of the fullerene [60] structure

2. Quantum mechanics I

Analysis of quantum mechanical postulates - pictures and representations; properties of sets of functions, operators and related theorems; degeneracy, spread of observation and uncertainty principle; Schmidt orthonormalisation; Fourier transformation, delta function with examples, free particle normalization, matrix formulation, bound states, the Virial theorem

3. Nanotechnology: principles and practices

Density of states – zero dimensional solid, one dimensional quantum wire, thin film and three dimensional box; some special nanomaterials – fullerenes, carbon nanotubes and nanodiamonds; optical properties of metallic and semiconducting nanoparticles; nanolithography

4. Thermodynamics and statistical mechanics

Legendre transformation with applications; Maxwell-Boltzmann distribution with degeneracy (for both distinguishable and indistinguishable particles), partition function and its properties, interpretation of thermodynamic laws, thermodynamic function in terms of partition functions, molecular partition functions (translational, rotational, vibrational and electronic) for ideal gas, calculation of thermodynamic functions for monoatomic and diatomic gases, equipartition principle, equilibrium constant, theories of specific heat of solids

5. Atomic spectra

Elliptic orbits and space quantization; principal and azimuthal quantum numbers, total energy; orbital and spin angular momentum of electrons; vector model of atom, quantum numbers, orbital and spin angular momentum of electrons, normal and anomalous Zeeman and Paschenback effects, Stern-Gerlach experiment, Atomic energy terms and term symbols

6. Principles of molecular spectroscopy

Fundamentals; rotational spectra: intensity distribution, effect of non-rigidity on spectral features; vibrational spectra: potential energy of an oscillator, Harmonic Oscillator approximation, energy levels and selection rules, anharmonicity and its effect on energy levels and spectral features: overtones and hot bands, vibration-rotation spectra of diatomics: origin; selection rules; P, Q and R branches; Raman spectra: origin, selection rules, classical and quantum treatment of rotational and vibrational Raman spectra, resonance Raman spectroscopy; NMR spectra: theory, relaxation process, spin interactions - its origin, equivalent protons, qualitative idea of energy levels of AX, AX₂ and AX₃ systems, a few representative examples; Electronic spectra: Electronic absorption spectra of molecules, vibrational structures in electronic spectra, vibronic coupling: Herzberg Teller effect, Jahn-Teller effect, and Renner Teller Effect.

Recommended Books

S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.

V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.

D. M. Bishop, *Group Theory and Chemistry*, Oxford University Press, 1993.

A. K. Mukherjee and B. C. Ghosh, *Group Theory in Chemistry: Bonding and Molecular Spectroscopy*, Universities Press (India) Private Ltd., Hyderabad, 2018

A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.

- F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.
- L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.
- H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.
- P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
- L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.
- A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
- F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.
- R. Taylor, *The Chemistry of Fullerenes*, Advanced Series in Fullerenes, Vol 4, World Scientific, Singapore, 1995.
- D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt Ltd, New Delhi, 2003.
- C. N. R. Rao, A. Müller, A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis, Properties and Applications*, Vols 1 and 2, Wiley-VCH, Weinheim, 2004.
- C. Bréchnignac, P. Houdy, M. Lahmani, *Nanomaterials and Nanochemistry*, Springer, London, 2006.
- I. N. Levine, *Physical Chemistry*, Tata McGraw-Hill, New Delhi, 1978.
- K. Denbigh, *Principles of Chemical Equilibrium*, Cambridge University Press, Cambridge, 1981.
- I. M. Klotz and R. M. Rosenberg, *Chemical Thermodynamics*, John Wiley, New York, 1994.
- G. W. Castellan, *Physical Chemistry*, 3rd Edn, Narosa Publishing House, 1995.
- N. A. Gokcen and R. G. Reddy, *Thermodynamics*, Plenum Press, New York, 1996.
- G. K. Vemulapalli, *Physical Chemistry*, Prentice-Hall, India, 1997.
- P. W. Atkins, *Physical Chemistry*, Oxford University Press, Oxford, 1998.
- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.
- H. E. White, *Introduction to Atomic Spectra*, McGraw-Hill Kogakusha Ltd., Tokyo, 1934.
- G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill International Book Company, Tokyo, 1982.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, 4th Edn, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.
- J. D. Graybeal, *Molecular Spectroscopy*, McGraw-Hill International Editions, Spectroscopy series, 1998.
- D. A. McQuarrie and J. D. Simon, *Molecular Thermodynamics*, University Science Books, California, 1999.

MSCH105: Inorganic General**Practical Marks: 50, Credit: 4**

1. Experiments on quantitative estimation: analysis of selected ores, minerals and alloys
2. Synthesis and characterization of inorganic and coordination compounds: selected simple salts, double salts and coordination compounds with some common inorganic and organic ligands
3. Identification of some less common ions

MSCH106: Nuclear-Analytical General**Practical Marks: 50, Credit: 4**

1. Separation of ions involving ion exchange technique
2. Titrimetric estimation of different compounds
3. Beer's law: application in different chemical matrices

Semester-II (Total Marks 300, Credit: 24)**Core Subject****MSCH201: Inorganic General II****Marks: 50, Credit: 4**

1. Chemistry of elements and their compounds

Elements – structural versatility and related properties; compounds – design and syntheses, isolation, characterization, solution structure, molecular aggregate, crystalline architecture, spectral, magnetic and catalytic properties and application in chemistry, biology and materials science

Non-transition and transition metal ion homoleptic/ heteroleptic and homonuclear/ heteronuclear complexes of different dimensions with varied mono- and polydentate blockers containing carbon, nitrogen, phosphorus, chalcogen, halogen donors with/without mono-/polydentate bridges and counter ions

Chemistry of lanthanoids and actinoids: valence orbitals, general trends in chemistry, absorption spectroscopy, fluorescence behavior, antenna effect and quantum cutting, magnetic properties, chemical shift reagents, and neo-coordination chemistry

2. Cluster compounds

Clusters in elemental states, cluster classification, skeletal electron (Elm) counting, higher boron hydrides-structures and reactions, equation of balance, Lipscomb topological diagrams, polyhedral

skeletal electron pair theory (PSEPT), carboranes, metalloboranes and heteroboranes, metallocarboranes, zintl ions, Chevrel compounds, infinite metal chains, multidecker molecules, cluster-surface analogy.

3. Structure and properties of solids

Fundamentals, ionic, covalent, hydrogen bonded and molecular solids; perovskite, ilmenite and rutile; spinel and inverse spinel, diamond cubic, silicates: single/double chain, 3D network, pyroxene, amphibole, talc, mica, clay, zeolite; crystal defects, non-stoichiometric compounds; electronic properties of solids, F-centre, conductors, insulators, semiconductors, superconductors; ferroelectricity, antiferroelectricity, pyroelectricity, piezoelectricity, liquid crystals, cooperative magnetism.

Recommended Books

J. D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall, London, 1991.

G. Wulfsberg, *Principles of Descriptive Inorganic Chemistry*, University Science Books, Mill Valley, CA, 1991.

A. F. Holleman and E. Wiberg, *Inorganic Chemistry*, Academic Press, New York, 1995.

N. N. Greenwood and A. Earnshaw, *Chemistry of the Elements*, 2nd Edn, Pergamon, New York, 1997.

F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley & Sons, Inc, New York, 1999.

G. Wulfsberg, *Inorganic Chemistry*, Viva Books Pvt Ltd, New Delhi, 2001.

B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3rd Edn, John Wiley & Sons, Inc, New York, 2001.

P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry*, 4th Edn, Oxford, 2006.

J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structures and Reactivity*, 4th Edn, Pearson, New Delhi, 2006.

R. Xu, W. Pang and Q. Huo (Eds), *Modern Inorganic Synthetic Chemistry*, Elsevier, New York, 2011.

J. Crowe, T. Bradshaw and P. Monk, *Chemistry of Biosciences*, Oxford University Press, Oxford, 2006.

G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edn, Pearson, New Delhi, 2009.

J. R. Anderson and M. Boudart (Eds), *Catalysis: Science and Technology*, Springer, London, 2012.

G. Cao, *Nanostructures & Nanomaterials, Synthesis, Properties & Applications*, Imperial College Press, London, 2004.

L. Cademartiri and G. A. Ozin, *Concepts of Nanochemistry*, Wiley-VCH, Weinheim, 2009.

D. L. Kepert, *Inorganic Stereochemistry*, Springer, Berlin, 1982.

A. von Zelewsky, *Stereochemistry of Coordination Compounds*, Wiley, New York, 1996.

S.P. Sinha, *Systematics and Properties of Lanthanides*, Riedel, Dordrecht, 1983.

- J. J. Katz, G. T. Seaborg and L. R. Morss (Eds), *The Chemistry of the Actinide Elements*, Vols I and II, 2nd Edn, Chapman and Hall, London, 1986.
- G.B. Richter-Addo and P. L. Legzdins, *Metal Nitrosyls*, Oxford University Press, New York, 1992.
- F.A. Cotton and R. A. Walton, *Multiple Bonds Between Metal Atoms*, 2nd Edn, Clarendon Press, Oxford, UK, 1993.
- G.A. Jefferey and W. Saenger, *Hydrogen Bonding in Biological Structures*, Springer, Berlin, 1991.
- A.J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press, Oxford, 1996.
- G. A. Jeffrey, *An Introduction to Hydrogen Bonding*, Oxford University Press, Oxford, 1997.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley and Sons, New York, 2009.
- P. Powell, *Principles of Organometallic Chemistry*, 2nd Edn, Chapman and Hall, London, 1988.
- R. A. van Santen and M. Neurock *Molecular Heterogenous Catalysis*, Wiley-VCH, Weinheim, 2006.
- G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, International 2nd Edn, Oxford University Press, Oxford, 2010.
- I. Pelant and J. Valenta, *Luminescence Spectroscopy of Semiconductors*, Oxford, New York, 2012.
- D. M. P. Mingos and D. J. Wales, *Introduction to Cluster Chemistry*, Prentice Hall, New York, 1990.
- D. F. Shriver, H. D. Kaesz and R. D. Adams (Eds), *The Chemistry of Metal Cluster Complexes*, VCH, New York, 1990.
- C. E. Housecroft, *Cluster Molecules of the p-Block Elements*, Oxford University Press, Cambridge, 1994.
- K. J. Klabunde, *Free Atoms, Clusters and Nanoscale Particles*, Academic Press, New York, 1994.
- D. M. P. Mingos (Ed.), *Structural and Electronic Paradigms in Cluster Chemistry*, Springer, Berlin, 1997.
- P. Braunstein, L. A. Oro and P. R. Raithby (Eds), *Metal Clusters in Chemistry*, Wiley-VCH, Weinheim, 1999.
- M. Driess and H. Noth (Eds), *Molecular Clusters of the Main Group Elements*, Wiley-VCH, Weinheim, 2004.
- T. P. Fehlner, J. -F. Halet and J. -Y. Saillard, *Molecular Clusters - A Bridge to Solid State Chemistry*, Cambridge University Press, Cambridge, 2007.
- C. E. Housecraft and A. G. Sharpe, *Inorganic Chemistry*, 3rd Edn, Pearson Education Ltd, Essex, England, 2008.
- A. F. Wells, *Structural Inorganic Chemistry*, 5th Edn, Oxford University Press, Oxford, 1984.
- W. A. Harrison, *Electronic Structure and the Properties of Solids: The Physics of the Chemical Bonds*, Dover Publications, New York, 1989.
- D. M. Adams, *Inorganic Solids*, Wiley, New York, 1992.
- T. C. W. Mak and G. -D. Zhou, *Crystallography in Modern Chemistry*, Wiley, New York, 1992.
- S. R. Elliot, *The Physics and Chemistry of Solids*, JohnWiley & Sons, Chichester, 1998.

M. Cox, *Optical Properties of Solids*, Oxford University Press, Oxford, 2001.

L. E. Smart and E. A. Moore, *Solid State Chemistry: An Introduction*, 4th Edn, CRC Press, Boca Raton, FL, 2012.

A. R. West, *Solid State Chemistry and Its Application*, 2nd Edn, Wiley-VCH, Weinheim, 2014.

MSCH0202: Nuclear-Analytical General II

Marks: 50, Credit: 4

1. Nuclear properties and structure II:

Liquid drop model, formulation of semi-empirical binding energy equation, mass parabola and application of binding energy equation; nuclear reactions, Q-value and cross section of nuclear reaction, compound nucleus theory (qualitative approach), calculation of fission probability using binding energy equation, shell model, nuclear magic number and its derivation from nuclear potential well, calculation of nuclear spin, nuclear isomerism and non-optical transitions

2. Cosmochemistry

Different geological systems, age of rocks and earth, cosmic rays and its effect in meteorites, comets, black hole, nuclear reactions in stars, solar neutrino hypothesis

3. Synthetic elements

Man-made elements: theoretical background, production and separation with special reference to actinoids and super heavy elements, separation chemistry

4. Separation techniques

Chromatography: chromatogram, mathematical relations of capacity, selectivity factor, distribution coefficient, retention time; band broadening, column efficiency; column resolution, numerical problems, gas chromatography, high performance chromatography. Ionic liquids: synthesis, properties and applications, green solvent, capillary electrophoresis: principles, methods and applications

5. Electroanalytical methods I

Electrochemical cell, electrodes: reference and indicator electrodes, membrane electrodes, electrode-solution interface layer, gas-sensing probe, electrolytic process, three electrode system; supporting electrolyte, DME; Cottrell equation, Ilkovic equation, Ilkovic-Heyrofsky equation, test of reversibility, current-voltage diagram, DC and AC polarography, stripping voltammetry, amperometric titration

Recommended Books

B. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice Hall, New York, 1965.

- R. D. Evans, *The Atomic Nucleus*, McGraw-Hill, New York, 1979.
- G. R. Choppin and J. Rydberg, *Nuclear Chemistry: Theory and Applications*, Pergamon Press, Oxford, 1980.
- G. Friedlander, J. W. Kennedy, E. S. Macias and J. M. Miller, *Nuclear and Radiochemistry*, 3rd Edn, Jhon Wiley & Sons Inc., New York, 1981.
- G. Seaborg, *Modern Alchemy*, World Scientific, Singapore, 1994.
- H. J. Arnikaar, *Essentials of Nuclear Chemistry*, 4th Edn Reprint, New Age International (P) Ltd Publications, New Delhi, 2001.
- D. D. Sood, A.V. R Reddy and N. Ramamoorthy, *Fundamentals of Radiochemistry*, Yancas, Mumbai, 2004.
- W. D. Loveland, D. J. Morrissey and G. T. Seaborg, *Modern Nuclear Chemistry*, Wiley Interscience, New Jersey, 2006.
- D. D. Clayton, *Principles of Stellar Evolution and Nucleosynthesis*, Chicago University Press, Chicago, 1983.
- K. Heyde, *Basic Ideas and Concepts in Nuclear Physics*, IOP, Briston, 1999.
- G. R. Choppin, J. O. Liljenjin and J. Rydberg, *Radiochemistry and Nuclear Chemistry*, Butterworth-Heinmann, Woburu, 2002.
- Y. Marcus and A. S. Kertes, *Ion Exchange and Solvent Extraction of Metal Complexes*, Wiley Interscience, New Jersey, 1969.
- E. Heftman, *Chromatography*, Reinhold, New York, 1969.
- H. F. Walton and W. Reiman, *Ion Exchange in Analytical Chemistry*, Pergamon Press, Oxford, 1970.
- J. A. Dean, *Chemical Separation Methods*, Van Nostrand Reinhold, London, 1970.
- D. G. Peters, J. M. Hayes and G. M. Hieftje, *Chemical Separations and Measurements: Theory and Practice of Analytical Chemistry*, Saunders, Wiley Interscience, New York, 1974.
- D. A. Skoog, D. M. West and F. J. Holley, *Fundamentals in Analytical Chemistry*, 5th Edn, Saunders, Philadelphia, 1988.
- A. Tarter, *Advanced Ion Chromatography*, Wiley Interscience, New York, 1989.
- S. Lindsay and J. Barnes, *High Performance Liquid Chromatography*, John Wiley, New York, 1992.
- G. D. Christian, *Analytical Chemistry*, 5th Edn, Wiley, New York, 1994.
- S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, Wiley Eastern Ltd., New Delhi, 1998.
- D. R. Crow, *Polarography of Metal Complexes*, Academic Press, London, 1979.
- A. J. Bard and L. F. Faulkner, *Electrochemical Methods—Fundamentals and Applications*, 2nd Edn, Wiley, New York, 1998.
- C. G. Zoski (Ed) *Handbook of Electrochemistry*, Elsevier, New York, 2007.
- Ed. By R.Kellner, J.-M.Mermet, M.Otto, M.Valcarcel, H.M.Widmer, *Analytical Chemistry*, Wiley-VCH

MSCH203: Organic General II**Marks: 50, Credit: 4**

1. Reaction intermediates

General methods of generation, detection, stability, reactions and structure of classical and non-classical carbocations and carbanions; free radicals including radical cations and radical anions; carbenes; arynes and nitrenes; neighbouring group participation

2. Carbohydrates

Introduction, synthesis and protecting groups: esters, ethers, acetals, amines, etc; Reactions of monosaccharides: halogenation, alkene and carbocycle formation, anhydro sugars, deoxy and aminodeoxy sugars, miscellaneous; Disaccharide formation: chemical and enzymatic; chemical glycobiology

3. Organic spectroscopic analysis I

¹H NMR spectroscopy: Introduction, chemical shift, magnetic anisotropy, spin-spin coupling, tree-diagrams, germinal and vicinal couplings, homoallylic and allylic couplings, First-order and Non-first-order spectra, Pople notation, solvents, chemical exchange, chemical shift reagents, NOE

Mass Spectrometry: Instrumentation; Vaporization and Ionization process: EI, CI, ESI, MALDI etc.; Fragmentation process; Mass Analysis; Mass spectral data: Isotope peaks, Mass accuracy; Hyphenated mass spectral methods: GC-MS, LC-MS; MS-MS

4. Identification of organic compounds by spectroscopic techniques
(UV-VIS, FT-IR, NMR and Mass)

Recommended Books

J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 5th Edn, John Wiley, New York, 1999.

S. P. McManus, *Organic Reactive Intermediates*, Academic Press, New York, 1973.

F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry Part A and Part B*, 4th Edn, Plenum Press, New York, 2001.

T. L. Gilchrist and C. W. Rees, *Carbenes, Nitrenes and Arynes*, Nelson, New York, 1973.

T. H. Lowry and K.C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn, Harper and Row, New York, 1998.

Robert V. Stick, *Carbohydrates: The Sweet Molecules of Life*, Academic press, 2001

I. L. Finar, *Organic Chemistry*, Vol I, 6th Edn, Addison Wesley Longmann, London, 1998.

I. L. Finar, *Organic Chemistry*, Vol II, 5th Edn, ELBS, London, 1995.

- W. J. I. Noble, Highlights of Organic Chemistry, MerceL Dekker, New York, 1974.
- D. L. Nelson and M.M. Cox, Lehninger: Principles of Biochemistry, W.H. Freeman Co, London, 2005.
- W. J. I. Noble, Highlights of Organic Chemistry, MerceL Dekker, New York, 1974.
- E. A. Davidson, Carbohydrate Chemistry, Holt, Rinehart and Winston, New York, 1967.
- R. D. Guthrie and J. Honeyman, An Introduction of Chemistry of Carbohydrate, 3rd Edn, Clarendon Press, Oxford, 1988.
- J. Kennedy, Carbohydrate Chemistry, Clarendon Press, Oxford, 1988.
- R. T. Morison, and R. N. Boyd, Organic Chemistry, 6th Edn, Prentice-Hall India Pvt Ltd, New Delhi, 1992.
- J. R. Dyer, Applications of Absorption Spectroscopy of Organic compounds, 2nd print, Prentice Hall, New Jersey, 1971.
- R. C. Banks, E.R. Matjeka and G. Mercer, Introductory Problems in Spectroscopy, Benjamin/Cumings Publishing Co, 1980.
- W. Kemp, Organic Spectroscopy, 3rd Edn, McMillan, Hong Kong, 1991.
- R. M. Silverstein and F. Webster, Spectrometric Identification of Organic Compounds, 6th Edn, John Wiley, New York, 1998.
- D. H. Williams and I. Fleming, Spectroscopic Methods in Organic Chemistry, 5th Edn, Tata McGraw-Hill, New Delhi, 2005.
- D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, Spectroscopy, Brooks/Cole, a part of Cengage Learning, 2008.
- K. Biemann, Mass Spectrometry – Application to Organic Chemistry, McGraw-Hill, New York, 1962.
- H. Budzikiewicz, C. Djerassi and D.H. Williams, Mass Spectrometry of Organic Compounds, Holden-Day, 1967.
- J. Barker, Mass Spectrometry, 2nd Edn, John Wiley, New York, 2000.
- C. Dass, An Introduction to Biological Mass Spectrometry, Wiley, New York, 2002.
- K. Downard, Mass Spectrometry: A Foundation Course, Royal Society of Chemistry, UK, 2004.
- G. Siurdek, The Expanding Role of Mass Spectrometry in Biotechnology, MCC Press, San Diego, 2004.

MSCH204: Physical General II

Marks: 50, Credit: 4

1. Symmetry and group theory II

The Great Orthogonality Theorem: statement and interpretation, proof of important corollaries; construction of character tables, cyclic groups and construction of their character tables, direct product groups, direct product representations, projection operators (without derivations) and vanishing of integrals, invariance of the Hamiltonian operator and eigenfunctions of Hamiltonian operator (H) as bases of irreducible representations, SALCs and their use in calculating π MOs under the Hückel approximations for some simple systems, outlines of symmetry aspects of molecular spectra

2. Quantum mechanics II

Equation of motion, constants of motion; Ehrenfest's theorem, exactly solvable problems: step potential and tunneling, bound states, the Virial theorem, harmonic oscillator, rigid rotator; elementary discussion of the H-atom solution

3. Electrochemistry

Introduction, ion-solvent interaction: Born model and Born equation, enthalpy, entropy and free energy of ion-solvent interaction and their calculations, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant, factors responsible for ion association; effect of ion association over conductivity; ion-dipole and ion-quadrupole interactions; electrode kinetics: relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation and its importance; Hydrogen electrode and its application in charge transfer reaction.

4. Chemical kinetics

Theories of reaction rates: applications to uni-, bi- and termolecular reactions, thermodynamic formulation of reaction rate, reactions in solution cage effect, diffusion and activation controlled reactions (elementary idea), dielectric effect on ion-ion reaction, electrostriction, volume of activation, effect of pressure on reaction rate, classification of reactions on the basis of volume of activation, study of fast reactions flow process and relaxation techniques; Curtin-Hammett principle, linear free energy relationship, Hammett and Taft equations

5. Crystal structure

Crystal symmetry, translation, glide plane and screw axis, Bravais lattice, space groups and its determination, stereographic projection, Fourier series, electron density and structure factor, methods for solving the phase problems, B-zones and Fermi level in lattice, concept of particle-hole in conduction process, band theory, theory of conductors, semiconductors and insulators.

Recommended Books

- S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.
- V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.
- D. M. Bishop, *Group Theory and Chemistry*, Oxford University Press, Oxford, 1993.
- A. K. Mukherjee and B. C. Ghosh, *Group Theory in Chemistry: Bonding and Molecular Spectroscopy*, Universities Press (India) Private Ltd., Hyderabad, 2018
- A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.
- L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.
- D. Bohm, *Quantum Theory*, Asia Pub. House, Bombay, 1960.
- J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, London, 1961.
- L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.
- P. C. W. Davies, *Quantum Mechanics*, ELBS, London, 1985.

- P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
- A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
- F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.
- S. Glasstone, *An Introduction to Electrochemistry*, D. Van Nostrand Company, 1962.
- J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Vol I, Plenum Press, New York, 1970.
- G. W. Castellan, *Physical Chemistry*, 3rd Edn, Narosa Publishing House, New Delhi, 1995.
- R. A. Alberty and R. J. Silbey, *Physical Chemistry*, 1st Edn, John Wiley & Sons, Inc, New York, 1995.
- R. S. Berry, S. A. Rice and J. Ross, *Physical Chemistry*, Oxford University Press, Oxford, 2000.
- K. J. Laidler, *Reaction Kinetics*, Vols I and II, Pergamon Press, London, 1970.
- L.P. Hammett, *Physical Organic Chemistry*, McGraw-Hill Book Company, New Delhi, 1970.
- J. Albery, *Electrode Kinetics*, Oxford Chemistry Series, Clarendon Press, Oxford, 1975.
- K.J. Laidler, *Chemical Kinetics*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1988.
- M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, 1999.
- G. D. Mahan, *Many Particle Physics*, Kluwer Academy, Plenum Publisher, 2000.
- C. Kittel, *Introduction to Solid State Physics*, 4th Edn, John Wiley & Sons, New York.
- P. A. Cox, *The Electronic Structure & Chemistry of Solids*, Oxford University Press, Oxford, 1987.
- M. F. C. Ladd and R. A. Palmer, *Structure Determination by X-ray Crystallography*, 3rd Edn, Plenum Press, New York, 1994.
- W. Clegg, *Crystal Structure Determination*, Oxford University Press, Oxford, 2005.

Practical Papers

MSCH205: Organic General Practical

Marks: 50, Credit: 4

1. Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components

MSCH206: Physical General Practical

Marks: 50, Credit: 4

1. Experiments in kinetics
2. Experiments in equilibrium
3. Instrumental methods: potentiometry, polarimetry, colorimetry and conductometry
4. Data processing and elementary numerical techniques

Semester-III (Total Marks 300 Credit: 24)

Core Subject

MSCH301: Advanced Inorganic General

Marks: 50, Credit: 4

1. Reaction mechanism

Factors governing the rate of a chemical reaction, analysis of rate data, complex rate laws, kinetically indistinguishable schemes, nucleophilicity and rate scales: Edward scale, n_{Pt} scale, Gutmann donor number, Drago E & C scale, trans- and cis- effects, water exchange rates, proton ambiguity, mechanistic simulation; associative, dissociative, interchange, nucleophilic, electrophilic pathways; Hammett relation, application of LFER in chemical kinetics

2. Metal ion promoted reactions
Fundamentals, simple cycle, catalytic cycle, pliancy of substrates, Tolman catalytic loop, homogeneous/heterogeneous catalysis: Wacker-Smidt synthesis, Monsanto acetic acid process, hydrogenation by Wilkinson's catalyst, water gas shift reaction (WGSR), Fischer-Tropsch synthesis, hydrosilation, hydrophosphilylation, hydroamination, hydrocyanation and hydroboration reactions

2. Metal ion promoted reactions

Fundamentals, simple cycle, catalytic cycle, pliancy of substrates, Tolman catalytic loop, homogeneous/heterogeneous catalysis: Wacker-Smidt synthesis, Monsanto acetic acid process, hydrogenation by Wilkinson's catalyst, water gas shift reaction (WGSR), Fischer-Tropsch synthesis, hydrosilation, hydrophosphilylation, hydroamination, hydrocyanation and hydroboration reactions

3 Surfactants and polymers in aqueous solution

Adsorption at interfaces, aggregation, amphiphilic, plentiful in nature, raw materials, classification, dermatological aspects, ecological impact, biodegradation, surfactant development, surfactant micellization, phase behaviour of concentrated surfactant systems, physiochemical properties of surfactant and polymers containing oxyethylene groups, mixed micelles, intermolecular interactions, colloidal forces, polymers in solutions, regular solution theory, novel surfactants, surface active polymers, surfactant-polymer systems, surfactant-protein mixtures, natural surfactant

4. Atomic spectrometry in inorganic analysis

AAS, AES, AFS, ICP-AES, ICP-MS: Theory, instrumentation and application; electrothermal atomization, cold vapour and hydride generation techniques.

5. Molecular magnetism I

Different magnetic materials, van Vleck equation and its application, Curie-Weiss law and its implication, Lande interval rule, microstates, multiplet, multiplet width, hole formalism, zero-field splitting, spin-orbit coupling, quenching of orbital contribution, Fermi contact and pseudo-contact shifts, chemical shift reagent

6. Supramolecular Chemistry

New horizon and scientific/technological landscape, building blocks, atomic and molecular valences, supramolecular orbitals, pallet of non-covalent forces and harnessing them, supramolecular arrays, structure directed synthesis, deliberate isolation of different functional materials.

Recommended Books

J. O. Edwards and W. A. Benjamin, *Inorganic Reactions Mechanism*, INC, New York, 1965.

C. H. Langford and H. B. Gray, *Ligand Substitution Processes*, W. A. Benjamin, New York, 1966.

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

D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley & Sons, New York, 1987.

R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.

R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, Oxford, 1998.

J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, Wiley-VCH, Weinheim, 1997.

M. B. Wright, *Fundamental Chemical Kinetics—An Explanatory Introduction to the Concepts*, Harwood Publishing, Chichester, 1999.

S. Asperger, *Chemical Kinetics and Inorganic Reaction Mechanisms*, 2nd Edn, Springer, London, 2012.

G. W. Parshall, *Homogeneous Catalysis*, Wiley, New York, 1980.

C. N. Satterfield, *Heterogeneous Catalysis in Practice*, McGraw-Hill, New York, 1980.

O. N. Temkin, *Homogeneous Catalysis with Metal Complexes: Kinetic Aspects and Mechanisms*, John Wiley & Sons, New York, 2012.

M. Beller, A. Renken and R. A. van Santen, *Catalysis*, Wiley, New York, 2012.

Y. Moroi, Micelles, *Theoretical and Applied Aspects*, Plenum Press, New York, 1992.

M. M. Rieger and L. D. Rheis (Eds), *Surfactants in Cosmetics*, Marcel Dekker Inc, New York, 1997.

K. Holmberg, B. Jonsson, B. Kronberg and B. Lindman, *Surfactants and Polymers in Aqueous Solution*, John Wiley & Sons, New York, 2002.

M. N. Khan, *Micellar Catalysis*, Taylor and Francis Group, New York, 2007.

T. F. Tadros (Ed), *Emulsion Science and Technology*, Willey-VCH, Verlag GmbH and Co, 2009.

- G. Currell, *Analytical Instrumentation: Performance, Characteristics and Quality*, Wiley India Pvt Ltd, New Delhi, 2002. D. A. Skoog, D. M. West, F. J. Holler, S. R. Crouch, *Fundamentals of Analytical Chemistry*, Brooks/Cole CENGAGE Learning, New Delhi, 2004.
- G. D. Christian, *Analytical Chemistry*, 6th Edn, Wiley-India, New Delhi, 2004.
- M. Koel and M. Kaljurand, *Green Analytical Chemistry*, RSC Publishing, Cambridge, 2010.
- O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.
- P. Day and A. E. Underhill (Eds), *Metal-organic and Organic Molecular Magnets*, RSC, London, 2000.
- P. M. Lathi (Ed), *Magnetic Properties of Organic Materials*, Marcel Dekker, New York, 1999.
- J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, V; Molecule-based Magnets*, Wiley-VCH, Weinheim, 2005.
- F. E. Mabbs and D. J. Machin, *Magnetism and Transition Metal Complexes*, Dover Publications, New York, 2008.
- R. Winpenny (Ed), *Single-Molecule Magnets and Related Phenomena*, Structure and Bonding Series, Vol 122, Springer, Berlin, 2010.
- B. D. Cullity and C. D. Graham, *Introduction to Magnetic Materials*, 2nd Edn, John Wiley & Sons, New York, 2011. D. Gatteschi, R Sessoli and J. Villain, *Molecular Nanomagnets*, Oxford University Press, Oxford, 2006.
- R. Hilzinger and W. Rodewald, *Magnetic Materials*, Wiley, New York, 2013
- F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.
- V. Balzani and F. Scandola, *Supramolecular Photochemistry*, Ellis Horwood, Chichester, 1991.
- J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, Weinheim, 1995.
- G. A. Jeffrey, *An Introduction to Hydrogen Bonding*, Oxford University Press, Oxford, 1997.
- S. T. Hyde, B. Ninham, S. Anderson, Z. Blum, T. Landh, K. Larsson and S. Liddin, *The Language of Shape*, Elsevier, Amsterdam, 1997.
- C. N. R. Rao, A. Muller and A. K. Cheetham, *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH, Weinheim, Germany, 2007.
- C. C. Koch, *Nanostructured Materials Processing, Properties, and Applications*, William Andrew Inc, 2007.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.
- K. Rurack and R. Martinez-Manez (Eds), *The Supramolecular Chemistry of Organic-Inorganic Hybrid Materials*, John Wiley & Sons, Hoboken, New Jersey, 2010.
- E. R. T. Tiekink and J. Zukerman-Schpector (Eds), *The Importance of Pi-Interactions in Crystal Engineering: Frontiers in Crystal Engineering*, 1st Edn, John Wiley & Sons, Chichester, 2012.

1. Complexes in aqueous solution

Stability constants of metal complexes: determination by pH-potentiometric, spectrophotometric methods (slope-ratio, mole-ratio and Job's method of continuous variation), Bjerrum method, determination of composition, factors influencing stability of metal complexes, evaluation of thermodynamic parameters.

2. Advanced spectroscopic methods:

Instrumentation, presentation of spectra, Applications of heteronuclear NMR spectroscopy; ^{11}B , ^{14}N , ^{17}O , ^{19}F and ^{31}P -NMR, ^{195}Pt . CD/ORD: molecular dissymmetry and chiroptical properties, Cotton effect, magnetic circular dichroism (MCD), vibrational circular dichroism (VCD), applications. EPR: anisotropy, intensity, hyperfine splitting, Kramer's theorem, photoelectron spectroscopy, ESCA, UPS, Auger, AES, XRF and EXFAS; Synergistic benefit: spectroscopic and other tools in structure elucidation

3. Surface chemistry

Nanomaterials: definition, importance, classification, 0D, 1D, 2D structures – size effects, the general methods for the synthesis of nanostructures (sol-gel method, co-precipitation, microemulsion, solvothermal, sonochemical reaction etc), Solution growth techniques of 1D-2D nano structures: Synthesis of metallic, semiconducting and oxide nanoparticles – homo- and hetero-nucleation growth methods – template-based synthesis, different characterization techniques (XRD, TEM, SEM, AFM, XPS, Raman study etc) and their application

4. Mossbauer spectroscopy

Mossbauer effect - conditions, nuclear recoil, Doppler effect, instrumentation, chemical shift examples, quadrupole effect, effect of magnetic field, effect of simultaneous electric and magnetic fields, typical spectra of iron and tin compounds, NQR

5. Electroanalytical methods II

Cyclic voltammetry, differential pulse voltammetry, coulometry, electrogravimetry, LSV; methods, choice of solvent, supporting electrolyte, working electrode, switching potential, electrode potential, pathways of electron transfer: EEE, ECE; electro-induced reactions; conventional secondary batteries: Ni-Cd, Ni-Fe, Ag-Zn, ZEBRA system

Recommended Books

- R. M. Smith and A. F. Martell, *Critical Stability Constants*, 6 Vols, Plenum Press, New York, 1974-89.
 M. Meloun, J. Havel and E. Hogfeldt, *Computation of Solution Equilibria: A Guide to Methods in Potentiometry, Extraction and Spectrophotometry*, Halsted, New York, 1988.

- A. E. Martell and R. J. Motekaitis, *Determination and use of Stability Constants*, 2nd Edn, VCH, New York, 1992.
- J. G. Grasselli, M. K. Snavely and B. J. Bulkin, *Chemical Application of Raman Spectroscopy*, Wiley, New York, 1981.
- W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, Hong Kong, 1986.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.
- J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.
- K. Nakanishi and N. Berova, *Circular Dichroism, Principles and Applications*, VCH, New York, 1994.
- H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.
- J. A. Iggo, *NMR Spectroscopy in Inorganic Chemistry* (Oxford Chemistry Primers), 2003.
- A. K. Brisdon, *Inorganic Spectroscopic Methods* (Oxford Chemistry Primers), Oxford University Press, (Indian Edn), 2005.
- L. Kevan and R. N. Schwartz (Eds), *Time Domain Electron Spin Resonance*, John Wiley, New York, 1979.
- J. E. Wertz and J. R. Boulton, *Electron Spin Resonance: Elementary Theory and Practical Applications*, Chapman and Hall, London, 1986.
- N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.
- D. W. Turner, C. Baker and C. R. Bundle, *Molecular Photoelectron Spectroscopy*, Wiley Interscience, New York, 1970.
- J. H. D Eland, *Photoelectron Spectra*, Butterworth, London, 1984.
- T. L. Barr, *Modern ESCA: the Principles and Practice of X-ray Photoelectron Spectroscopy*, CRC Press, Boca Raton, FL, 1994.
- D. P. Woodruff and T. A. Delchar, *Modern Techniques of Surface Science*, Cambridge University Press, Cambridge, 1988.
- T. Thomson, M. D. Baker, A. Christie and J. F. Tyson, *Auger Electron Spectroscopy*, John Wiley, New York, 1985.
- G.A. Ozin, A. C. Arsenault and L. Cademartiri, *Nanochemistry: A Chemical approach to Nanomaterials*, Royal Society of Chemistry, London, 2009.
- V. I. Goldanskii and R. H. Herber, *Chemical Applications of Mossbauer Spectroscopy*, Academic Press, New York, 1968.
- N. N. Greenwood and T. C. Gibb, *Mossbauer Spectroscopy*, Chapman and Hall, London, 1971.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.

J. M. Hollas, *Modern Spectroscopy*, Wiley, New York, 1996.

D. R. Crow, *Polarography of Metal Complexes*, Academic Press, London, 1979.

A. J. Bard and L. F. Faulkner, *Electrochemical Methods—Fundamentals and Applications*, 2nd Edn, Wiley, New York, 1998.

C. G. Zoski (Ed), *Handbook of Electrochemistry*, Elsevier, New York, 2007.

MSCH303: Advanced Organic General

Marks: 50, Credit: 4

1. Organic photochemistry I

Photochemical energy, Jablonski diagram, photosensitisation and quenching, Norrish Type-I and Type-II processes, Paterno-Buchi reaction, photochemistry of unsaturated compounds: *cis/trans*-isomerization

2. Pericyclic reaction I

Definition, classification, cyclo-additions and cyclo-reversion reactions, [2+2], [2+4], [4+6] reactions, catalysis; dipolar cyclo-additions; ene reactions; regioselectivity, stereo-selectivity and stereo-specificity in pericyclic reactions

3. Reactions with cyclic intermediates or cyclic transition states

Introduction, stereochemical control via tethering: Robinson annelation, iodolactonisation, synthesis of *trans*-fused ring; sulfur as a tether, cyclic transition states

4. Oxidation and Reduction

Oxidations: alcohol to carbonyl (activated DMSO, DMP, TPAP, Mukaiyama oxidation, Metal based reagents, etc), epoxidation, dihydroxylation, C-H oxidation, miscellaneous; Reductions: carbonyl group, hydrogenation, electron transfer

Recommended Books

R. B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Verlag Chemie GmbH, 1970.

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

I. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, John Wiley, New York, 1980.

T. H. Lowry and K. C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn, Harper and Row, New York, 1998.

H. O. House, *Modern Synthetic Reactions*, 2nd Edn, Benjamin, 1971.

W. Caruthers, Modern Methods of Organic Synthesis, 3rd Edn, Cambridge University Press, Cambridge, 1996.

J. Clayden, N. Greeves, S. Warren, and P. Wothers, Organic Chemistry, Oxford University Press, Oxford, 2001.

O. L. Chapman, Some Aspects of Organic Photochemistry, Dekker, 1967. J. M. Coxon and B. Halton, Organic Photochemistry, Cambridge University Press, Cambridge, 1974.

R. O. C. Norman and J. M. Coxon, Principles of Organic Synthesis, 3rd Edn, ELBS, 2003.

J. Singh and J. Singh, Photochemistry and Pericyclic Reactions, 3rd Edn, New Age International (P) Ltd, India, 2012.

A. Griesbeck, M. Oelgemoller and F. Ghetti, Organic Photochemistry and Photobiology, 3rd Edn, Vol I, CRC Press, Boca Raton, FL, 2012.

F. D. King, Medicinal Chemistry: Principles And Practice, 2nd Edn, Royal Society of Chemistry, 2002.

G. L. Patrick, An Introduction to Medicinal Chemistry, 3rd Edn, Oxford University Press Inc, New York, 2005.

A. Kar, Medicinal Chemistry, 4th Edn, New Age International (P) Ltd, India, 2007.

C. G. Wermuth, The Practice of Medicinal Chemistry, 3rd Edn, Academic Press, New York, 2008.

MSCH 304-M (GE) Basics in Medicinal Chemistry

Marks: 25, Credit: 2

Organic and Inorganic medicinal compounds and their mode of action, natural and synthetic organic compounds, Inorganic metal complexes, Organometallic compounds as medicines Radio-pharmaceuticals: pharmaceuticals for diagnostic, pathological and clinical treatment, radionuclides, generator systems, separation of carrier free radionuclides for labeling, tomography, ^{18}F FDG, PET, SPECT, RIA.

Recommended Books

Medicinal chemistry 4/E Ashutosh Kar, New Age International Pub.

An Introduction to medicinal chemistry 3/E Graham L. Patrick, Oxford (International student Edn.)

Medicinal Inorganic chemistry, Edited by J. L. Sessler, S. R. Doctrow, T. J. McMurry and S. J. Lippard, American chemical society, Washington, DC.

(Instant Notes) Medicinal chemistry, G. Patrick, Viva Books Pvt. Ltd.

Medicinal chemistry Principles and practice, 2/E, edited by F. D. King, Royal Society of Chemistry.

Medicinal Chemistry, D. Sriram & P. Yogeewari, Pearson.

MSCH 304-I (GE) Basics in Industrial Chemistry

Marks: 25, Credit: 2

Fuels and Combustion: Definition, calorific value, solid, liquid and gaseous fuels, petrochemicals, nuclear fuels, bio-fuels

Polymers: Preparation, types, characterization, molecular weight determination, uses

Glass and ceramics: Clays, silica, methods of fabrication of different wares, porcelain and vitreous enamels

Analytical tools and techniques: UV-Vis, IR, AAS, Fluorescence, NMR, Mass spectroscopy, Analysis of analytical data

Recommended Books

Principles and practice of analytical chemistry, F. W. Fifield & D. Keatey, Blackwell publishing.

Fundamentals of analytical chemistry, 5 Koog, West, Hollert Crouch, Thomson Books.

Analytical chemistry 6/E G. D. Christian, J. Willey.

Chemical Analysis: An Instrumental Approach, A K. Srivastava & P. C. KJain, S. Chand & Co.

Organic spectroscopy 3/E, W. Kemp, PALGRAVE Publishers.

Applications of absorption spectroscopy of organic compounds, John R. Dyer, PHI learning Pvt. Ltd.

Spectrometric indentificatio of Organic compounds, 4/E, Silverstain, Bassler and Morrill, John wiley & sons.

Spectroscopy, D. L. Pavia, G. M. Lampman, G. S. Kriz & J. R. Vyvyan, CENGAGE learning.

Industrial chemistry, R. K. Das

Indystruak aookucatuibs if radui usitioes abd raduatuibm edutirs S. M. Rao, A. B. Majali, R. G. Derhpande & T. S. Murthy.

MSCH 305-I (DE) Inorganic Major-I**Marks: 50, Credit: 4**

1. Synthetic methodology for inorganic, coordination and organometallic compounds

Different synthetic protocols: thermal, photochemical, sonochemical, solvothermal, electrochemical; self-assembly; green synthesis: solvent free synthesis, microwave assisted synthesis, reactions in ionic liquids, atom economy; suitable synthesis for C-H activation, CO₂ fixation, water oxidation; synthesis of suitable higher valent metal complexes in catalysis

2. Organometallic chemistry II

Reactions that occur at the metal: Ligand substitution, oxidative addition, reductive elimination; Reactions involving modification of ligands: Insertion and deinsertion, Nucleophilic addition to the ligand, nucleophilic abstraction, electrophilic reactions; Applications to organic synthesis: enantioselective functional group interconversion, chiral synthesis, protection and deprotection; transmetallation and cyclisation reactions, metallo-fullerenes, bioorganometallics, organo-lanthanoids and actinoids, organo-dendrimer, surface organometallic chemistry

3. Spectral (IR, NMR, EPR, UV-Vis, Mossbauer, etc.) studies of inorganic, coordination and organometallic species Fundamentals, elucidation of geometric structure, electronic structure, stereochemistry, bonding, molecular aggregate, superstructure and reaction pathway in halide, pseudohalide, carbonyl, nitrosyl, DMSO, polypyridine, azoheterocycle, oxime, quinone, macrocycle containing compounds and organometallic complexes; enumeration and characterization: geometrical (*cis/trans, fac/mer*) and stereo (optical) isomers in different polyhedra; ligational motif and chelate loop, structural distortion, effective pi-acceptance centre, oxidation state, spin state, redox site of non-innocent ligands, mu-bonding and hapticity, electrophilicity/nucleophilicity, quasi- and superaromaticity, fluxionality, metalloligand, probing chemical reactivity and reaction pathways (intramolecular/intermolecular, stereoretentivity/stereodynamicity), covalency of ML bonding, comment on bonding theories and structure-function relationships

Recommended Books

L. S. Hegedus, *Transition Metal in the Synthesis of Complex Organic Molecules*, University Science Press, Mill Valley, CA, 1994.

F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6th Edn, John Wiley & Sons, Inc, New York, 1999.

G. Wulfsberg, *Inorganic Chemistry*, Viva Books Private Ltd, New Delhi, 2001.

W. Carruthers and I. Coldham, *Modern Methods of Organic Synthesis*, 4th Edn, Cambridge University Press, Cambridge, 2004.

G. Rothenberg, *Catalysis: Concepts and Green Applications*, Wiley-VCH, Weinheim, 2008.

- H. -D. Höltje, W. Sippl, D. Rognan and G. Folkers, *Molecular Modeling: Basic Principles and Applications*, 3rd Edn, Wiley-VCH, Weinheim, 2008.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.
- R. Xu, W. Pang and Q. Huo (Eds), *Modern Inorganic Synthetic Chemistry*, Elsevier, New York, 2011.
- E. Abel, F. G. A. Stone and G. Wilkinson (Eds) *Comprehensive Organometallic Chemistry*, Vols 1-8, Pergamon Press, Oxford, 1980-1995.
- A. Yamamoto, *Organotransition Metal Chemistry*, Wiley, New York, 1986.
- J. P. Collmann, L. S. Hegedus, J. R. Norton and R. G. Finke, *Principles and Applications of Organotransition metal Chemistry*, University Science Books, Mill Valley, CA, 1987.
- R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
- R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 2nd Edn, Wiley, New York, 1994.
- L. S. Hegedus, *Transition Metal in the Synthesis of Complex Organic Molecules*, University Science Press, Mill Valley, CA, 1994.
- G. O. Spessard and G. L. Miessler, *Organometallic Chemistry*, Prentice-Hall, New Jersey, 1997.
- R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, Oxford, 1998.
- M. Periasamy, *Organic Synthesis Using Iron-Carbonyl Reagents*, *Curr. Sci.*, 2000, 78, (11), 1307-1313
- R. V. Eldik and C. D. Hubbard (Eds) *Advances in Inorganic Chemistry*, Vol 54, Academic Press, New York, 2003.
- R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 4th Edn, Wiley, New York, 2005.
- D. Steinborn, *Fundamentals of Organometallic Catalysis*, John Wiley & Sons, New York, 2011.
- G. Aruldas, *Molecular Structure and Spectroscopy*, 2nd Edn, Prentice-Hall of India, New Delhi, 2007.
- D. N. Sathyanarayana, *Electronic Absorption Spectroscopy and Related Techniques*, University Press, 2001.
- D. Shillady, *Essentials of Physical Chemistry*, CRC Press, Boca Raton, FL, 2012.
- R. S. Drago, *Physical Methods in Inorganic chemistry*, Saunders, Philadelphia, 1977.
- C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.
- A. B. P Lever, *Inorganic Electronic Spectroscopy*, Elsevier, New York, 1984.
- C. Trindle and D. Shillady, *Electronic Structure Modeling: Connection between Theory and Software*, CRC Press, Boca Raton, FL, 2008.
- D. N. Sathyanarayana, *Vibrational Spectroscopy Theory and Applications*, New Age International, New Delhi, 1996.
- H. H. Jaffe and M. Orchin, *Symmetry, Orbitals and Spectra*, Wiley, New York, 1982.
- B. E. Douglas and C. A. Hollingsworth, *Symmetry in Bonding and Spectra, An Introduction*, Academic Press, New York, 1985.
- K. Nakamoto, *Infrared and Raman Spectra of Inorganic and Coordination Compounds*, Part B, 6th Edn, John Wiley & Sons, New Jersey, 2009.
- B. Schrader (Ed) *Infrared and Raman Spectroscopy: Methods and Applications*, VCH Weinheim, 1995.
- W. Henderson and J. S. McIndoe, *Mass Spectrometry of Inorganic, Coordination and Organometallic Compounds:*

Tools-Techniques-Tips, John Wiley & Sons, Ltd, Chichester, 2005.

A. E. Derome, *Modern NMR Techniques in Chemical Research*, Pergamon Press, Oxford, 1987.

W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, 1986.

J. K. M. Sanders, E. C. Constable and B. K. Hunter, *Modern NMR Spectroscopy: A Workbook of Chemical Problems*, Oxford University Press, Oxford, 1993.

H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.

A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Metal Ions*, Clarendon Press, Oxford, 1970.

N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.

W. O. George and H. O. Willis, *Computer Methods in Ultraviolet, Visible and Infra-red Spectroscopy*, Royal Society of Chemistry, 1990.

E. A. V. Ebsworth, D. W. H. Rankin and S. Craddock, *Structural Methods in Inorganic Chemistry*, 2nd Edn, Blackwell Scientific Publications, Oxford, 1991.

F. Gerson, *High Resolution ESR. Spectroscopy*, John Wiley, New York, 1971.

J. E. Wertz and J. R. Boulton, *Electron Spin Resonance: Elementary Theory and Practical Applications*, Chapman and Hall, London, 1986.

J. Garcia Sole, L. E. Bausa and D. Jaque, *An Introduction to the Optical Spectroscopy in Inorganic Solids*, John Wiley & Sons, New York, 2005.

MSCH 305-N (DE) Nuclear Analytical Major-I

Marks: 50, Credit: 4

1. Elementary particles and radioactive decay

Early discoveries, fundamental interactions, classification of conservation laws and symmetries, standard model, quarks, families of matter, beyond the standard model, accelerators

2. Radioactive disintegration

Alpha decay paradox and its explanation in terms of tunnel effect, Geiger-Muller relationship, Golden rule and its application in explaining beta and gamma transition, selection rules

3. Nuclear reactions

General features, types of nuclear reaction, conservation laws, nuclear reaction dynamics, mechanism of nuclear reaction, use of uncertainty principle, resonance and non-resonance reaction, optical model and calculation of mean free path, nuclear fission and fusion reaction, calculation of fission probability from Bohr-Wheeler's theory Centre of mass system and laboratory co-ordinate, optical model.

4. Nuclear detectors

Mechanisms of interaction between electrons & matter, synchrotron radiation, Mu-meson, Range-Energy relation for mono-energetic electrons, Photoelectric and Compton effect, Pair-production, interaction of neutrons with matter, radiative capture, different types of scintillators like inorganic and organic or liquid, liquid scintillators and their applications, scintillation mechanism, working principle of semiconductor detectors--- some applications, gas-filled detectors—principle of operation and applications, G-M and proportional counters, classification of nuclear detectors, variation of amplitude vs. voltage - characterization of different zones, role of quench gases - limitations of proportional detectors: proportional counter performance, flow-type proportional counter, gas multiplication factor, space charge effects.

5. Coincidence counting

Determination of absolute disintegration rates, decay scheme studies

6. Green analytical chemistry (GAC)

Challenges in the GAC, greening sample preparation techniques, membrane extraction, microwave assisted, ultrasound and ionic liquid assisted extraction, pressurized and supercritical fluid extraction; green chromatography separation, green solvents - water, ionic liquids, polyethylene glycol, fluoros, miniaturization of analytical devices, solid-phase micro and nano - extraction, passive methods of analysis, Green analytical detection methodologies; green electrochemistry, waste minimization

Recommended Books

- J. M. Blatt, V. F. Weissleopf, *Theoretical Nuclear Physics*, Wiley, New York, 1952.
 G. M. Mayer and J. H. D. Jensen, *Elementary Theory of Nuclear Shell Structure*, Wiley, New York, 1955.
 D. Holliday, *Introductory Nuclear Physics*, Wiley, New York, 1955.
 L. R. B. Elton, *Nuclear Sizes*, Oxford University Press, Oxford, 1961.
 I. Kaplan, *Nuclear Physics*, Addison-Wesley, Cambridge, 1963.
 B. Harvey, *Introduction to Nuclear Physics and Chemistry*, Prentice-Hall, New York, 1965.
 M. Haissinsky, *Nuclear Chemistry Audits Application*, Addison Wesley, 1965.
 M. Lefort, *Nuclear Chemistry*, D. Van Nostrand, London, 1968.
 B. L. Cohen, *Concepts of Nuclear Physics*, McGraw-Hill, New York, 1971.
 R. D. Evans, *The atomic nucleus*, McGraw-Hill, New York, 1979.
 G. F. Knoll, *Radiation Detection and Measurements*, John Wiley & Sons, New York, 1979.
 G. Friedlander, E. F. Macias, J. W. Kennedy and J. M. Miller, *Nuclear and Radiochemistry*, Wiley Interscience, New York, 1981.
 R. Eisberg and R. Resnick, *Quantum Physics of Atoms, Molecules, Nuclei and Particles*, 2nd Edn, John Wiley & Sons, New York, 1985.
 S. S. Kapoor and V. S. Ramamurthy, *Nuclear Radiation Detections*, New Age International, New Delhi, 1986.
 W. R. Leo, *Techniques of nuclear and particle physics experiments*, Narosa Publishing House, 1995.
 H. J. Arnikaar, *Nuclear Chemistry through Problems*, 4th Edn, New Age International, New Delhi, 1995.
 S. B. Patel, *Nuclear Physics*, New Age International, New Delhi, 1996.
 G. Choppin, J. O. Lilienzin and J. Rydberg, *Radiochemistry and Nuclear Chemistry*, Butterworth-Heinemann, 2001.
 H. J. Arnikaar, *Essentials of Nuclear Chemistry*, New Age International, 4th Edn, New Delhi, 2001.
 G. Friedlander, J. W. Kennedy, B. S. Macias and J. M. Miller, *Nuclear and Radiochemistry*

MSCH 305-O (DE) Organic Major-I**Marks: 50, Credit: 4**

1. Organometallics

Bonding in transition metal; organometallic complexes; some common properties of organometallic complexes; fluxionality, stabilisation of reactive or unstable molecules; catalytic hydrogenation, insertion reactions; organo-Cu, -Zn, -Cd, -Hg and -Pd compounds; metallocenes (Fe, Ru, Os); carbene and carbyne complexes

2. Terpenes

Structural studies on sesquiterpenes, diterpenes, triterpenes and carotenoids; chemistry of carryophyllene, abietic acid, β -amyrin, α and β -carotenoids

3. Organic spectroscopic analysis

^{13}C NMR spectroscopy: Introduction, chemical shifts, proton-coupled and -decoupled ^{13}C NMR spectrum, off-resonance decoupling, heteronuclear coupling: C-F and C-P, NOE effect, DEPT experiment, application in structure elucidation, 2D-NMR

Applications of CD/ORD in structure elucidation, octant rule, axial halo ketone rule, lactone sector rule

4. Stereo selective reactions of carbonyl compounds and alkenes

Carbonyls: nucleophilic addition using chiral- substrates, auxiliaries, reagents and catalysts; reactions at α -carbon: enolate formation; enolate alkylation; use of chiral auxiliaries: oxazolidinone, oxazoline, etc.; aldol reaction, asymmetric aldol reaction

Alkenes: hydrogenation, epoxidation; conjugate addition; allyl and crotyl boranes

5. Controlling the geometry of double bonds:

Wittig reaction of stabilized and unstabilized ylide, Julia olefination, Peterson elimination, etc.

Recommended Books

J. Tsujiz, Organic Synthesis by Means of Transition Metal Complexes, Springer-Verlag, New York, 1975.

E. Abel, F. G. A. Stone and G. Wilkinson, Comprehensive Organometallic Chemistry, Vols 3-10, Pergamon Press, Oxford, 1980-1995.

G. Davies, Organo Transition Metal Chemistry: Application in Organic Synthesis, Pergamon Press, Oxford, 1982.

J. Pearson, Metalloorganic Chemistry, 1985.

J. P. Collman and S. L. Hegedus, Principles and Applications of Organo-Transition Metal Chemistry, University Science Book, Mill Valley, 1986.

A. Yamamoto, Organo-Transition Metal Chemistry, John Wiley, New York, 1986.

R. H. Crabtree, The Organometallic Chemistry of Transition Metals, 2nd Edn, John Wiley, New York, 1994.

R. C. Mehrotra and A. Singh, Organometallic Chemistry : A Unified Approach, 2nd Edn, New Age International Pvt Ltd, India, 2000.

A. F. Hill, Organotransition Metal Chemistry, Royal Society of Chemistry, London, 2002.

- P. De Mayo, *The Higher Terpenoids*, Interscience Publishers, 1959.
- A. R. Pinder, *The Chemistry of Terpenes*, Chapman and Hall, 1960.
- K. Nakanishi, T. Goto, S. Ito, S. Natori, and S. Nozoe, *Natural Products Chemistry*, Vol. I (1974) and Vol. II (1975), Academic Press, New York.
- S. Hanessain, *Total Synthesis of Natural Products: The Chiron Approach*, Pergamon Press, Oxford, 1984.
- I. L. Finar, *Organic Chemistry*, Vol II, 5th Edn, ELBS, London, 1995.
- K. J. Hale, *The Chemical Synthesis of Natural Products*, Sheffield Academic Press/CRC Press, Boca Raton, FL, 2000.
- E. Breitmaier and W. Voelter, *¹³C NMR Spectroscopy: Methods and Application in Organic Chemistry*, 3rd Edn, Verlag Chemie, 1987.
- M. Duer (Ed), *Introduction to Solid State NMR Spectroscopy*, Blackwell, 2004.
- T. D. W. Claridge, *Tetrahedron Organic Chemistry Series Volume 19, High-Resolution NMR Techniques in Organic Chemistry*, Pergamon, Oxford, 2004.
- D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, *Spectroscopy*, Brooks/Cole, a part of Cengage Learning, 2008.
- P. Deslongchamps, *Stereoelectronic Effect in Organic Chemistry*, Pergamon Press, Oxford, 1983. R. S. Atkinson, *Stereoselective Synthesis*, Wiley, New York, 1995.
- K. C. Nicolson and E. J. Sorensen, *Classics in Total Synthesis*, VCH, Weinheim, 1996.
- W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn, Cambridge University Press, Cambridge, 1996.
- T. H. Lowry and K. C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn, Harper and Row, New York, 1998.
- J. March, *Advanced Organic Chemistry: Reactions, Mechanism and Structure*, 5th Edn, John Wiley, New York, 1999.
- F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry, Parts A and B*, 4th Edn, Plenum Press, London, 2001.
- J. R. Hanson, *Organic Synthetic Methods*, Royal Society of Chemistry, London, 2002.
- R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3rd Edn, ELBS, London, 2003.
- E. M. Carreira, O. Rerser, *Classics in Stereoselective Synthesis*, John Wiley & Sons, New York, 2007.
- D. Nasipuri, *Stereochemistry of Organic Compounds*, 2nd Edn, Wiley Eastern, New Delhi, 1993.
- E. L. Eliel, S.H. Wilen and L.N. Mander, *Stereochemistry of Organic Compounds*, John Wiley & Sons, New York, 1994.
- K. Nakanishi and N. Berova, *Circular Dichroism, Principles and Applications*, VCH, New York, 1994.

MSCH 305-P (DE) Physical Major-I

Marks: 50, Credit: 4

1. Thermodynamics of irreversible processes

Limitations of classical (equilibrium) thermodynamics, entropy production in some simple irreversible processes, the concept of forces and fluxes, linear phenomenological relations; Onsager reciprocity relation - derivation from fluctuation theory; Curie-Prigogine principle - statement and proof using one scalar and one vector forces, illustrations; Saxen's relations in connection with electrokinetic phenomena and their proof using Onsager reciprocity relations, stationary states: variation of entropy production with time, Prigogine's criterion for establishment of stationary state, applicability of Le Chatelier's principle on stationary states

2. Kinetics

Introduction, autocatalysis, chain reactions: branched and non-branched kinetic rate equations, Semenov treatment for branched chain reactions; explosion: population explosion, upper and lower ignition/explosion limits; thermal ignition and ignition temperature; chemical oscillation: some models (Lotka, Oregonator and Brusselator); analysis of Lotka and Brusselator model, conditions for oscillation, chemistry of BZ reaction (Brusselator model); theories of unimolecular reactions: Lindemann, Hinshelwood, RRK and RRKM

3. Symmetry and group theory III

Construction of SALCs and their use in calculating π MOs under the Hückel approximations, (ii) calculation of MOs of AB_n type and sandwich type molecules, (iii) study of hybridization, selection rules, allowedness/forbiddenness of $n-\pi^*$ and $\pi-\pi^*$ transitions, (iv) splitting of terms in octahedral and tetrahedral ligand fields, Orgel and Tanabe-Sugano diagrams, (v) symmetry aspects of molecular vibrations - infrared and Raman activity, conservation of orbital symmetry in pericyclic reactions

4. Photochemistry

Radiative and non-radiative processes, fluorescence and phosphorescence: temperature and pressure effect; delayed fluorescence and triplet-triplet annihilation; mirror image relationship, quantum yield, life-time and δ -pulse response, ICT state with examples; phenomenological approach of quenching, transient effects; properties of excited states: dipole moment, pK_a by Förster method, energy transfer, photoinduced electron transfer, excimers and exciplexes; special photochemical reactions, flash photolysis, laser flash photolysis

Recommended Books

- I. Prigogine, *Introduction to Thermodynamics of Irreversible Processes*, Interscience Publishers, 1967.
 V. N. Kondrat'ev, *Chemical Kinetics of Gas Reactions*, Pergamon Press, 1964.
 P. C. Jordan, *Chemical Kinetics and Transport*, John Wiley & Sons, Inc, New York, 1979.
 K. J. Laidler, *Chemical Kinetics*, TMH Publishing Company Limited, 1988.
 S. K. Scott, *Oscillations, Waves, and Chaos in Chemical Kinetics*, Oxford University Press, Oxford, 1994.
 M. J. Pilling and P. W. Seakins, *Reaction Kinetics*, Oxford University Press, Oxford, 1995.
 M. R. Wright, *Fundamental Chemical Kinetics*, Horwood Publishing, Chichester, 1999.
 E. Kreyszig, *Advanced Engineering Mathematics*, 5th Edn, Wiley Eastern, New Delhi, 1988.
 G. Arfken, *Mathematical Methods for Physicists*, Academic Press, New York, 1966.
 M. K. Jain, *Numerical Methods for Scientific and Engineering Computation*, Wiley Eastern Ltd, New Delhi.
 R. A. McQuarrie and J. D. Simons, *Physical Chemistry* 1st Edn, Viva Books Private Limited, New Delhi, 1998.
 S. C. Rakshit, *Molecular Symmetry Group and Chemistry*, The New Book Stall, Kolkata, 1988.
 V. Heine, *Group Theory in Quantum Mechanics: An Introduction to Its Present Usage*, Dover Publication, New York, 1991.
 R. D. M. Bishop, *Group Theory and Chemistry*, Dover Publications Inc, New York, 1993.
 A. K. Mukherjee and B. C. Ghosh, *Group Theory in Chemistry: Bonding and Molecular Spectroscopy*, Universities Press (India) Private Ltd., Hyderabad, 2018
 A. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
 F. A. Cotton, *Chemical Applications of Group Theory*, 3rd Edn, John Wiley & Sons, New York, 1999.
 R. McWeeny, *Symmetry: An Introduction to Group Theory and Its Applications*, Dover Publications, New York, D. A. McQuarrie and J. D. Simon, *Molecular Thermodynamics*,

University Science Books, California, 1999. J. B. Buirks, *Photophysics of Aromatic Molecules*, Wiley-Interscience, New York, 1969.

P. W. M. Jacobs, *Group Theory with Applications in Chemical Physics*, Cambridge University Press, Cambridge, 2005.

K. K. Rohatgi-Mukherjee, *Fundamentals of Photochemistry*, New Age International (P) Limited, Publishers, India, 2007.

Practical papers

MSCH 306-I (DE) Inorganic Major-I Practical **Marks: 50, Credit: 4**

1. Quantitative analysis of major and minor components in ores and alloys by volumetric, complexometric, gravimetric and other instrumental methods after separation of the components by solvent extraction or chromatographic techniques
2. Chromatographic and ion-exchange separation of ions.
3. Visit to research institute/Industry

MSCH 306-N (DE) Nuclear-Analytical Major-I Practical **Marks: 50, Credit: 4**

1. Quantitative analysis of major, minor and trace components of ores and alloys by conventional and instrumental methods
2. Analysis of water, cement, fertilizer, food and drug
3. Visit to research institute/Industry

MSCH 306-O (DE) Organic Major-I Practical **Marks: 50, Credit: 4**

1. Different types of chromatographic techniques
2. Isolation of selected natural products
3. Visit to research institute/Industry

MSCH 306-P (DE) Physical Major-I Practical **Marks: 50, Credit: 4**

1. Experiments on surface chemistry: determination of CMC by conductometric, tensiometric, viscometric and spectrophotometric methods
2. Experiments on kinetics-II: variable temperature, experiments on equilibrium, micelles
3. Visit to research institute/Industry

MSCH 307 Social Outreach **Marks: 25, Credit: 02**

Students will take part in different social awareness program to be decided by the department time to time.

Semester-IV (Total Marks 300, Credit: 24)**Core Subject****MSCH401: Advanced Physical General****Marks: 50, Credit: 4**

1. Surface chemistry

Introduction, adsorption isotherms, surface excess; BET isotherm, LB film, membrane equilibrium, micellisation

2. Macromolecules

Introduction, average molecular weights and their determinations; Carothers' equation, kinetics of addition and condensation polymerization, flexibility of polymer chain, statistics of polymer dimensions and configurations, effect of solvent on the average dimensions; theories of polymer solutions: excluded volume and Flory-Huggins theory

3. Non-ideal systems

Virial equations, second Virial coefficient; London dispersion forces; determination of intermolecular potentials employing hard-sphere, square-well and hybrid potential models; non-ideal solutions; partial molar quantities and their determinations, Duhem-Margules equation and its applications, regular solutions and excess thermodynamic functions

4. Mathematics in Quantum Mechanics

Elementary vector calculus, equation of continuity of fluid motion, diagonalisation of square symmetric matrices (real elements) by Jacobi method; coordinate transformation the Jacobian and its use; Legendre, associated Legendre polynomials; Hermite polynomials; Lagurre and associated Lagurre polynomials; polynomials as orthonormal functions, their properties; complete solution of the H-atom problem

5. Spectroscopy

Transition between electronic states, principle of laser action, pump-probe spectroscopy, selection rules and forbidden transitions; NMR: relaxation and exchange phenomena, Overhauser effect, theories of chemical shift and nuclear spin-spin coupling in 2-spin systems with applications, pulsed NMR (spin echo); Electronic: $n-\pi^*$, $\pi-\pi^*$ and CT transitions; vibrational: simple polyatomic molecules, normal modes, influence of nuclear spin on vibration-rotation spectra of polyatomics

Recommended Books

R. C. Evans, *An Introduction to Crystal Chemistry*, 2nd Edb, Cambridge University Press, Cambridge, 1964.

- M. F. C. Ladd and R. A. Palmer, *Structural Determination by X-ray Crystallography*, 3rd Edn, Plenum, New York, 1994.
- D. P. Woodruff and T. A. Delchar, *Modern Techniques of Surface Science*, Cambridge University Press, Cambridge, 1988.
- W. Adamson, *Physical Chemistry of Surfaces*, John Wiley & Sons, New York, 1990.
- H. -J. Butt, K. Graf and M. Kappl, *Physics and Chemistry of Interfaces*, Wiley-VCH, 2003.
- J. H. Clint, *Surface Chemistry*, Blackie and Son Ltd, 1992.
- C. Tanford, *Physical Chemistry of Macromolecules*, John Wiley & Sons, Inc, New York, 1961.
- F. W. Billmeyer, *Text Book of Polymer Science*, 2nd Edn, Wiley-Interscience, New York, 1971.
- G. S. Mishra, *Introductory Polymer Chemistry*, Wiley Eastern, New Delhi, 1993.
- P. Ghosh, *Polymer Science and Technology of Plastic and Rubber*, Tata McGraw-Hill Publishing Company Limited, New Delhi, 1993.
- S. F. Sun, *Physical Chemistry of Macromolecules: Basic Principles and Issues*, John Wiley & Sons, New York, 1994.
- G. W. Castellan, *Physical Chemistry*, 3rd Edn, Narosa Publishing House, 1995.
- R. A. Alberty and R. J. Silbey, *Physical Chemistry*, 1st Edn, John Wiley and Sons, Inc, New York, 1995.
- I. N. Levine, *Physical Chemistry*, 4th Edn, Tata McGraw-Hill, New Delhi, 1995.
- L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.
- E. Merzbacher, *Quantum Mechanics*, John Wiley & Sons, New York, 1970.
- P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.
- L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.
- A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.
- F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.
- I. N. Levine, *Quantum Chemistry*, 4th Edn, Prentice Hall of India Pvt Ltd, New Delhi, 1995.
- G. M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill International Book Company, Tokyo, 1982.
- W. Kemp, *NMR in Chemistry: A Multinuclear Approach*, Macmillan Press, Hong Kong, 1986.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1992.
- J. K. M. Sanders, E. C. Constable and B. K. Hunter, *Modern NMR Spectroscopy: A Workbook of Chemical Problems*, Oxford University Press, Oxford, 1993.
- C. N. Banwell and E. M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw-Hill Publishing Company Ltd, New Delhi, 1994.
- H. Gunther, *NMR Spectroscopy: Basic Principles, Concepts and Applications in Chemistry*, Wiley, New York, 1995.
- A. Abragam and B. Bleaney, *Electron Paramagnetic Resonance of Transition Metal Ions*, Clarendon Press, Oxford, 1970.
- N. M. Atherton, *Principles of Electron Spin Resonance*, Ellis Horwood/Prentice-Hall, Hemel Hempsted, 1993.
- W. O. George and H. O. Willis, *Computer Methods in Ultraviolet, Visible and Infra-red Spectroscopy*, Royal Society of Chemistry, London, 1990.

Mechanism of energy and/ electron transfer process(es), various supramolecular devices: electronic, ionic and switching devices, application of supramolecular chemistry in photodynamic therapy, some examples of self-assembly in supramolecular chemistry with prospect in medicinal applications

2. Medicinal Chemistry and Drug Discovery

Antibacterial, Anticancer, Antitussive, and Antiviral agents; Opium analgesics, Antibiotics; New drugs from old poisons; Drug discovery, Structure-Activity Relationships (SARs)

3. Radiopharmaceuticals

Nuclear pharmacy: concept, pharmaceuticals and radiopharmaceuticals; type of radionuclides, neutral/charged particle emitters, radionuclide generators; ideal radiopharmaceuticals, methods of radiolabeling, biodistribution, specific radiopharmaceuticals for diagnostic and therapeutic purposes, SPECT, PET, ¹⁸F-FDG etc. method of administration, principle and instrumentation of gamma/PET camera for detection, quality control, Principle, method and application of radioimmunoassay(RIA).

4. Medicinal Inorganic Chemistry

Biomedical significance and inorganic chemistry, Characterization of biomolecules using spectroscopic methods, mechanistic aspects of heavy metal toxicity, platinum anti-cancer drugs (from laboratory to clinic), discovery and development of newer generation anti-tumour and anti-cancer agents

5. Pharmacokinetics

Drug absorption, drug distribution, drug metabolism, drug excretion, drug administration, drug dosing

6. Photodynamic medicine

Introduction, early days of photodynamic therapy (PDT), basic principle, photodynamic action, photochemotherapy, photosensitizing molecule, incubation period, light activation, light exposure, total light dose and its fluence rate, application of photosensitizer drug,

7. Drug Targets and Drug Delivery

Enzymes, receptors, carrier proteins, structural proteins, nucleic acids, lipids, carbohydrate, targeted drug delivery, novel delivery modalities, Future considerations

Recommended books

1. Radiopharmaceutical Chemistry, by Jason S. Lewis, Albert D. Windhorst, Brian M. Zeglis, Springer, 2019

2. Photodynamic Therapy: Basic Principles and Clinical Applications 1st Edition, by B.W. Henderson and T.J. Daugherty, ISBN-13: 978-0824786809, **CRC Press; 1 edition (June 19, 1992)**,

3. Radiopharmaceuticals for Therapy, by Ashutosh Dash and F. F. (Russ) Knapp, 2016, Springer
4. The Handbook of Radiopharmaceuticals, by Azuwuikwe Owunwanne, Mohan Patel and Samy Sadek, Chapman & Hall Medical, 1st Edition, 1995
5. Handbook of Radiopharmaceuticals: Radiochemistry and Applications, By M.J. Welch and C.S. Redvanly, Wiley, 2005
6. An Introduction to Medicinal Chemistry, Graham L. Patrick, Oxford (International Student Edition).
7. Medicinal Inorganic Chemistry, Edited by J.L. Sessler, s.R. Doctrow, T.J. Mcmurry and S.J. Lippard, American Chemical Society, Washington, DC.
8. (Instant Notes) Medicinal Chemistry, G. Patrick, Viva Books Pvt. Ltd.
9. Medicinal Chemistry, Principles and Practice, edited by F.D. King, Royal Society of Chemistry
10. The practice of Medicinal Chemistry, Edited by C.G. Wermuth, Academic Press.

MSCH403-I: Inorganic Major-II

Full Marks: 50, Credit: 4

1. Electrochemical studies of redox non-innocent ligands and metal complexes

Fundamentals, experimental findings of CV, DPV and coulometry, delving reversible, quasi-reversible and irreversible electrochemical and chemical processes in model compounds; electro-induced reactions: protic/electroprotic equilibrium, electrocatalysis, electro-polymerisation, electro-crystallisation, electro-chemiluminescence; electro-synthesis, evaluating comproportionation constant, OTTLE, surface-modified electrode, photo-electrochemistry, spectro-electrochemistry, excimer and its structure, excited state potential and chemical simulation, redox orbital, redox series, redox isomer, electron hopping, spatially isolated orbital; synergistic experiments and exposing electron transfer site, model case correlating biological processes

2. Redox reactions

General remark, complementary and non-complementary redox reactions, outer-sphere reaction, inner-sphere reaction, effect of bridging ligand in inner-sphere reaction, kinetics and mechanism, electron tunneling hypothesis, heteronuclear redox reaction and simplified Marcus theory; Marcus cross relationship and its application, remote attack, doubly-bridged process, ligand exchange, intervalence electron transfer, induced reaction, electron transport in biological systems and their simulations

3. Inorganic photochemistry

Preamble, photoexcitation, fluorescence, phosphorescence, photosensitization, quenching, charge and energy transfer, prompt and delayed reactions, excimer structure, substitution, fragmentation, isomerisation, exchange and redox reactions; chemiluminescence, photochromism; photochemistry using laser beams; chemical actinometry and determination of quantum yield, inorganic photochemistry in biological processes and their model studies; applications of photochemical reactions of coordination compounds - synthesis and catalysis, solar energy conversion and storage

4. Inorganic reaction mechanism

Substitution reactions in square planar, tetrahedral and octahedral geometries with special reference to d^n ion complexes: operational tests, aquation and anation, reactions without metal-ligand bond breaking, kinetics of chelate formation, reaction mechanisms of organometallic systems, studies on fast reactions, kinetic and activation parameters - tools to propose a plausible mechanism; stereochemical changes: types of ligand rearrangements, isomerism in 4-, 5- and 6-coordinated complexes; reactions of coordinated ligands: model choice of metal and ligand, acid-base reaction, hydrolysis of esters, amides and peptides, aldol condensation, trans-amination, template reactions, organic synthesis with special reference to macrocyclic ligand; reactions in fluxional organometallic compounds

Recommended Books

- J. O'M. Bockris and A. K. N. Reddy, *Modern Electrochemistry*, Plenum Press, New York, 1970.
- S. R. Morrison, *Electrochemistry in Semiconductor and Oxidised Metal Electrodes*, Plenum Press, New York, 1980.
- J. Koryta and K. Stulik, *Ion-selective Electrodes*, Cambridge University Press, Cambridge, 1983.
- A. J. Bard, R. Parsons and J. Jordan, *Standard Potentials in Aqueous Solution*, Dekker, New York, 1985.
- S. Torii, *Electro-Organic Syntheses*, Part I: *Oxidations*, Part II: *Reductions*, VCH, Weinheim, 1985.
- A. J. Fry and W. E. Britton (Eds), *Organic Electrochemistry*, Dekker, New York, 1985.
- E. Heitz and G. Kreysa, *Principles of Electrochemical Engineering*, VCH, Weinheim, 1986.
- D. E. Kyriacou and D. A. Jannakoudis, *Electrocatalysis for Organic Synthesis*, Wiley, New York, 1986.
- J. Goodisman, *Electrochemistry: Theoretical Foundations*, Wiley, New York, 1987.
- A. P. F. Turner, I. Karube and G. S. Wilson (Eds), *Biosensors: Fundamentals and Applications*, Oxford University Press, Oxford, 1987.
- R. J. Gale (Ed), *Spectroelectrochemistry: Theory and Practice*, Plenum Press, New York, 1988.
- M. I. Ismail (Ed), *Electrochemical Reactors: Their Science and Technology*, Elsevier, Amsterdam, 1989.
- J. Janata, *Principles of Chemical Sensors*, Plenum Press, New York, 1989.
- D. Pletcher and F. C. Walsh, *Industrial Electrochemistry*, 2nd Edn, Chapman and Hall, London, 1990.
- R. Varma and J. R. Selman (Eds), *Techniques for Characterization of Electrodes and Electrochemical Processes*, Wiley, New York, 1991.
- J. Koryta, *Ions, Electrodes, and Membranes*, Wiley, Chichester, 1991.
- J. O'M. Bockris and S. U. M. Khan, *Surface Electrochemistry*, Plenum Press, New York, 1993.
- C. M. A. Brett and A. M. O. Brett, *Electrochemistry: Principles, Methods and Applications*, Oxford University Press, Oxford, 1993.
- P. W. Atkins, *Physical Chemistry*, 5th Edn, Oxford University Press, Oxford, 1994.
- K. V. Kordesch, *Fuel Cells and Their Applications*, VCH, Weinheim, 1994.
- D. T. Sawyer, A. Sobkowiak and J. L. Roberts, Jr, *Experimental Electrochemistry for Chemists*, 2nd Edn, Wiley, New York, 1995.
- P. A. Christensen and A. Hammett, *Techniques and Mechanisms in Electrochemistry*, Blackie, Edinburgh, 1995.

- P. G. Bruce, *Solid-state Electrochemistry*, Cambridge University Press, Cambridge, 1995.
- F. Goodrich and K. Scott, *Electrochemical Process Engineering*, Plenum Press, New York, 1995.
- W. Schmickler, *Interfacial Electrochemistry*, Oxford University Press, Oxford, 1996.
- C. A. Vincent and B. Scrosati, *Modern Batteries*, 2nd Edn, Arnold, London, 1997.
- C. H. Hamann, A. Hamnett and W. Vielstich, *Electrochemistry*, Wiley-VCH, New York, 1998.
- A. J. Bard and L. F. Faulkner, *Electrochemical Methods—Fundamentals and Applications*, 2nd Edn, Wiley, New York, 1998.
- G. E. Marcelle, *Molten Salts: From Fundamentals to Applications*, Kluwer Academic Publisher, 2001.
- C. H. Hamann, A. Hamnett and W. Vielstich, *Electrochemistry*, Wiley-VCH, Weinheim, Germany, 2007.
- W. L. Reynolds and R. W. Lumry, *Mechanism of Electron Transfer*, Ronald Press, New York, 1966.
- H. Taube, *Electron Transfer Reaction of Complex Ions in Solution*, Academic Press, New York, 1970.
- P. Atkins, T. Overton, J. Rourke, M. Weller and F. Armstrong, *Shriver & Atkins Inorganic Chemistry*, 4th Edn, Oxford, 2006.
- G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3rd Edn, Pearson, New Delhi, 2009.
- C. J. Ballhausen, *Introduction to Ligand Field Theory*, McGraw-Hill, New York, 1962.
- B. N. Figgis, *Introduction to Ligand Field Theory*, Interscience, New York, 1966.
- S. C. Rakshit, *Molecular Symmetry Groups and Chemistry*, The New Book Stall, Kolkata, 1988.
- C. J. Ballhausen, *Molecular Electronic Structure of Transition Metal Complexes*, McGraw-Hill, London, 1979.
- V. Balzani and V. Carassiti, *Photochemistry of Coordination Compounds*, Academic Press, New York, 1970.
- A. W. Adamson and P. D. Fleischauer (Ed), *Concept of Inorganic Photochemistry*, Wiley, New York, 1975.
- G. L. Geoffroy and M. S. Wrighton, *Organometallic Photochemistry*, Academic Press, New York, 1970.
- A. R. Hollebone, C. H. Langford and N. Serpone, *Inorganic Photochemistry*, *Coord. Chem. Rev.*, 1981, 39, 181. D. Rendell and D. Mowthrope, *Fluorescence and Phosphorescence Spectroscopy*, John Wiley, New York, 1987.
- C. E. Wayne and R. P. Wayne, *Photochemistry*, Oxford University Press, 1st Indian Edn, New Delhi, 2005. J. R. Lakowicz, *Principles of fluorescence spectroscopy*, 3rd Edn, Springer, USA, 2006.
- M. sauer, J. Hofkens and J. Enderlein, *Handbook of Fluorescence Spectroscopy and Imaging: from Singles to Ensembles*, Wiley-VCH, Weinheim, Germany, 2011.
- J. O. Edwards and W. A. Benjamin, *Inorganic Reactions Mechanism*, INC, New York, 1965.
- C. H. Langford and H. B. Gray, *Ligand Substitution Processes*, W. A. Benjamin, New York, 1966.
- F. Basolo and R. G. Pearson, *Mechanism of Inorganic Reactions*, 2nd Edn, Wiley, New York, 1967.
- D. Katakis and G. Gordon, *Mechanisms of Inorganic Reactions*, John Wiley & Sons, New York, 1987.
- R. G. Wilkinns, *Kinetics and Mechanism of Reactions of Transition Metal Complexes*, 2nd Edn, VCH, Weinheim, 1991.
- R. B. Jordan, *Reaction Mechanisms of Inorganic and Organometallic Systems*, Oxford University Press, Oxford, 1998.
- J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2nd Edn, Wiley-VCH, Weinheim, 1997.
- S. Asperger, *Chemical Kinetics and Inorganic Reaction Mechanisms*, 2nd Edn, Springer, London, 2012.

1. Chemistry of exotic and hot atoms

Positron annihilation, probability of positronium formation, reaction and mechanism of positronium ion, chemistry of muonium and pionium ions; hot atom chemistry, Szilard-Chalmer reaction and retention of activity, primary and secondary retention, synthesis of labelled compounds

2. Applications of radiotracers

Isotope dilution; DIDA, IIDA and substoichiometric methods of analysis, application and numerical problems; nuclear activation analysis: principles, classifications and methods of nuclear activation analysis: principle, different types, interferences, K0 methods and comparative methods for analysis, special types of derivative activation analysis, depth profile activation analysis, cyclic activation analysis, secondary particle activation analysis; problems and applications, charged-particle activation analysis (CPAA): principles, calculation, applications, PGNA, PIXE, PIGE, IPAA, RBS; design of a new radiopharmaceutical: general considerations and factors; biosynthesis, factors in labeling: efficiency, isotope effect, storage conditions, radiolysis; specific methods of labeling; quality control; physicochemical and biological test

3. Chemical and biological effects of radiation

Ionizing radiation and its physical and chemical effect in target, water, radiolysis, (definition of different units in radiation chemistry, calculation of radiation dose, biological effects, source of human data, lethal dose, permissible level of radiation dose), primary radiological products of water and their characterization, dosimetric concepts and quantities, different types of chemical dosimeters, thermoluminescence and lyoluminescence and explanation - different unusual reactions by lyoluminescence

4. Nuclear reactor and accelerators

Nuclear energy vs. other forms of energies, India's nuclear energy program from Homi Bhabha, requirement of nuclear energy in Indian scenario: neglecting and justifying controversies. General features, types of reactor, carbides and nitrides as nuclear fuel substrate - their superiority, four-factor formula, charge particle accelerator, van de Graff generator, linear accelerator, cyclotron, synchrotron, synchrocyclotron, superconducting cyclotron, disposal of nuclear waste with specific reference to glass

Recommended Books

I. M. Kolthoff, P. J. Elving and E. B. Sandell, *Treatise on Analytical Chemistry*, Pt-I, II, III, The Interscience Encyclopedia, Inc, New York, 1959,

A. I. Vogel, *A Text Book of Quantitative Inorganic Analysis*, 3rd Edn, Longmans, London, 1961.

J. Green and J. Lee, *Positronium Chemistry*, Academic Press, New York, 1964.

J. W. T. Spinks and R. J. Woods, *An Introduction to Radiation Chemistry*, Wiley, New York, 1964.

- J. F. Duncan and G. B. Cook. *Isotopes in Chemistry*, Clarendon Press, Oxford, 1968.
 S. Ahrland, J. O. Liljerzin and J. Rydberg, *Chemistry of the Actinides*, Pergamon Press, Oxford, 1986.
 J. J. Katz, G. T. Seaborg and L. R. Morss (Eds), *Chemistry of the Actinide Elements*, Chapman and Hall, London, 1986. W. D. Ehmann and D. E. Vance, *Radiochemistry and Nuclear Methods of Analysis*, John Wiley, New York, 1991.
 J. Turner, *Atoms, Radiation and Radiation Protection*, Willey Interscience, New York, 1995.

MSCH403-O: Organic Major-II

Full Marks: 50, Credit: 4

1. Organic photochemistry II

Photochemical rearrangements: cyclohexenone, cyclohexadienone, dienone and β,γ -unsaturated systems, di- π -methane and aza di- π -methane rearrangements, photo induced substitution reaction in aromatic systems; photo- reduction and oxidation, photoaddition and photoisomerisation reactions

2. Alkaloids

Classification, general reactions of alkaloids, typical reactions, conversions and rearrangements of morphine and papaverine alkaloids

3. Heterocycles

Structure, synthesis and reactivity of 5,6-membered rings containing two heteroatoms, pyrimidines and purines

4. Organic synthetic process

Retrosynthetic analysis; C-C bond formation reactions; synthesis of L-Hexoses; Prostaglandins; Thienamycin; Biotin, etc

5. Spectroscopy and stereochemistry

NMR; determination of conformation and configuration in six-membered rings (3J variation with dihedral angle); stereochemistry of fused rings; spreading out effect: variation of vicinal coupling constant in cyclic compounds (3-6-membered rings), The π -contribution to geminal coupling; nuclear Overhauser effect

Recommended Books

- N. J. Turro, *Molecular Photochemistry*, Benjamin and Co, 1955.
 W. A. Noyes, G.S. Hammond and J. N. Pitts, *Advances in Photochemistry*, Vol I, Interscience Publisher, New York, 1964.
 O. L. Chapman, *Some Aspects of Organic Photochemistry*, Dekker, 1967.
 D. C. Neekers, *Mechanistic Organic Photochemistry*, Reinhold, New York, 1967.
 J. M. Coxon and B. Halton, *Organic Photochemistry*, Cambridge University Press, Cambridge, 1974.
 C. H. J. Wells, *Introduction to M.L. Photochemistry*, Chapman and Hall, London, 1974.
 J. Singh and J. Singh, *Photochemistry and Pericyclic Reactions*, 3rd Revised Edn, New Age International (P) Ltd, New Delhi, 2012.
 A. Griesbeck, M. Oelgemoller and F. Ghetti, *Organic Photochemistry and Photobiology*, 3rd Edn, Vol I, CRC Press, Boca Raton, FL, 2012.

- K. Nakanishi, T Goto, Sho Ito, S. Natori, and S. Nozoe, *Natural Products Chemistry*, Vol I (1974) and Vol II (1975), Academic Press, New York.
- K. W. Bentley, *The Alkaloids, Part II*, Interscience Publishers, New York, 1965.
- S. W. Pelletier, *Chemistry of the Alkaloids*, Van Nostrand Reinhold Co, 1970.
- J. A. Joule, K. Mills, *Heterocyclic Chemistry*, 5th Edn, John Wiley & Sons, Ltd, UK, 2010.
- R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley, New York, 1994.
- R. S. Atkinson, *Stereoselective Synthesis*, Wiley, New York, 1995.
- K. C. Nicolson and E. J. Sorensen, *Classics in Total Synthesis*, VCH, New York, 1996.
- W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn, Cambridge University Press, Cambridge, 1996.
- J. R. Hanson, *Organic Synthetic Methods*, Royal Society of Chemistry, London, 2002.
- R. S. Ward, *Selectivity in Organic Synthesis*, John Wiley & Sons, New York, 2003.
- C. Bolm, J. A. Gladysz, *Chemical Reviews* 2003, 103 (8).
- E. M. Carreira, O. Rerser, *Classics in Stereoselective Synthesis*, John Wiley & Sons, New York, 2007.
- D. L. Pavia, G. M. Lampman, G. S. Kriz and J. R. Vyvyan, *Spectroscopy*, Brooks/Cole, a part of Cengage Learning, 2008. W. Kemp, *Organic Spectroscopy*, 3rd Edn, McMillan, Hong Kong, 1991.
- D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 5th Edn, Tata McGraw-Hill, New Delhi, 2005.
- R. M. Silverstein and F. Webster, *Spectrometric Identification of Organic Compounds*, 6th Edn, John Wiley, New York, 1998.
- K. Biemann, *Mass Spectrometry – Application to Organic Chemistry*, McGraw-Hill, New York, 1962.
- H. Budzikiewicz, C. Djerassi and D. H. Williams, *Structure Elucidation of Natural Products by Mass Spectrometry*, Vol I and Vol II, Holden-Day, 1964.
- N. S. Bhacca, S. Norman and D. H. Williams, *Application of NMR Spectroscopy in Organic Chemistry*, Holden-Day, 1964.
- H. Budzikiewicz, C. Djerassi and D. H. Williams, *Mass Spectrometry of Organic Compounds*, Holden-Day, 1967.
- R. B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Verlag Chemie GmbH, 1970.
- K. Downard, *Mass Spectrometry: A Foundation Course*, Royal Society of Chemistry, London, 2004.
- C. Dass, *An Introduction to Biological Mass Spectrometry*, Wiley, New York, 2002.
- G. Siurdek, *The Expanding Role of Mass Spectrometry in Biotechnology*, MCC Press, San Diego, 2004.
- T. D. W. Claridge, *Tetrahedron Organic Chemistry Series Vol 19, High-Resolution NMR Techniques in Organic Chemistry*, Pergamon, Oxford, 2004.
- M. Duer (Ed), *Introduction to Solid State NMR Spectroscopy*, Blackwell, 2004.
- F. Hillenkamp, J. P. Katalinic, *A Practical Guide to MALDI MS: Instrumentation, Method and Applications*, 2006.
- T.L. Gilchrist, *Heterocyclic Chemistry*, 3/e, Pearson.

MSCH403-P: Physical Major-II

Full Marks: 50, Credit: 4

1. Classical mechanics

Classical equations of motion: Newton, Lagrange and Hamilton's forms, Poisson Bracket in classical mechanics, relation of Poisson Bracket's with commutators in quantum mechanics, phase space, Liouville's equation, microcanonical, scanonical and grand canonical ensembles

2. Statistical mechanics

Ensembles, statistical distribution and properties of distribution function, the H theorem and approach to equilibrium; Maxwell-Boltzmann (MB), Bose-Einstein (BE) and Fermi-Dirac (FD) distributions, the derivation of thermodynamic relations, thermodynamic and characteristic features of MB, BE and FD systems (ideal cases), black body radiation and photon gas; applications: (i) statistical thermodynamics of ideal systems (effect of nuclear spin and electronic angular momentum), (ii) specific heat of solids - Debye treatment, (iii) non-ideal gas

3. Electric and magnetic properties of matter

Dielectric polarization; Debye equation and its limitation; Onsager's reaction field model; electric polarizability of molecules; magnetic susceptibility - diamagnetic and paramagnetic, thermodynamic treatment of magnetic work; magnetic cooling; Curie law, superconductivity

4. Molecular interactions

Hamiltonian in absence and presence of external fields, forces in molecules, Hellmann-Feynmann theorem, perturbation treatment of electric polarisability, intermolecular interaction - calculation of dispersion energy, the London formula

Recommended Books

F. Reif, *Fundamentals of Statistical and Thermal Physics*, McGraw-Hill, New York, 1965.

E. S. R. Gopal, *Statistical Mechanics and Properties of Matter*, Ellis Horwood, England, 1974.

S. K. Ma, *Statistical Mechanics*, World Sci, Singapore, 1985.

R. K. Pathria, *Statistical Mechanics*, Butterworth-Heinemann, 1996.

P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.

F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New York, 1990.

A. J. Stone, *The Theory of Intermolecular Forces*, Clarendon Press, Oxford, 1996.

C. J. F. Böttcher, *Theory of Electric Polarisation*, Vols 1 and 2, Elsevier Scientific Publishing Co, New York, 1973. D. W. Davies, *The Electric and Magnetic Properties of Molecules*

MSCH404-I: Inorganic Major-III

Full Marks: 50, Credit: 4

1. Crystal Engineering

Crystal design and synthesis – an utmost need, general protocols, secondary building blocks, reticular approach, modular method, retrosynthetic strategy, supramolecular synthon, intermolecular forces, superstructure, molecular self-assembly, MOFs, crystal orbitals, cocrystals, polymorphism, property design

2. Inorganic materials

Molecules and crystals to materials, scaffold, art of synthesis, interwoven bonding, predictable crystalline architecture, intermolecular and interion interactions, dangling bond, surface pressure, surface functionalisation, core-corona, hysteresis, robust and directional interactions, click chemistry, functional materials: conducting, superconducting, magnetic, non-linear, porous, luminous, liquid crystals, quantum dots, catalysts, molecular and electronic devices, biosensors, biomineralization, proteomics, dendrimers, molecular recognition

3. Molecular magnetism II

Isolation of different molecular magnets, magnetic interactions in di- and polynuclear systems and clusters, cryogenic experiment, mechanism of exchange interaction, Bleaney-Bowers equation, antiferromagnetism (AF), ferromagnetism (F), single molecule magnet, deliberate synthetic approach of ferromagnetically coupled system, accidental orthogonality, spin canting, canted-AF, canted-F, spin frustration, admixed-spin, spinflop, metamagnetism, superparamagnetism, long-range ordering, calculation of ground state and spin manifold, magnetization versus field studies, inorganic, organic, metal-organic and organometallic magnetic materials

Recommended Books

- G. A. Jeffrey and W. Saenger, *Hydrogen Bonding in Biological Structures*, Springer, Berlin, 1991.
- P. L. Huyskens and T. Zeegers-Huyskens, *Intermolecular Forces: An Introduction to Modern Methods and Results*, Springer-Verlag, Berlin, 1991.
- G. R. Desiraju, J. J. Vittal, A. Ramanan, *Crystal Engineering: A text book*, IISc Press and World Scientific, 2011
- G. A. Jeffrey, *An Introduction to Hydrogen Bonding*, Oxford University Press, Oxford, 1997.
- E. R. T. Tiekink and J. Zukerman-Schpector (Eds), *The Importance of Pi-Interactions in Crystal Engineering: Frontiers in Crystal Engineering*, 1st Edn, John Wiley & Sons, Chichester, UK, 2012.
- S. T. Hyde, B. Ninham, S. Anderson, Z. Blum, T. Landh, K. Larsson and S. Liddin, *The Language of Shape*, Elsevier, Amsterdam, 1997.
- F. Vogtle, *Supramolecular Chemistry: An Introduction*, Wiley, Chichester, 1991.
- B. Dietrich, P. Viout and J. -M. Lehn, *Macrocyclic Chemistry—Aspects of Organic and Inorganic Supramolecular Chemistry*, VCH, Weinheim, 1993.
- J. -M. Lehn, *Supramolecular Chemistry: Concepts and Perspectives*, VCH, Weinheim, 1995.
- G. R. Newkome, C. N. Moorefield and F. Vogtle, *Dendritic Molecules*, VCH, Weinheim, 1996.
- G. R. Desiraju (Ed), *Crystal Design: Structure and Function, Perspectives in Supramolecular Chemistry*, Vol 7, Wiley, Chichester, 2003.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2nd Edn, John Wiley & Sons, New York, 2009.
- K. Rurack and R. Martinez-Manez (Eds), *The Supramolecular Chemistry of Organic-Inorganic Hybrid Materials*, John Wiley & Sons, Hoboken, New Jersey, 2010.

- R. Xu, W. Pang and Q. Huo (Eds), *Modern Inorganic Synthetic Chemistry*, Elsevier, New York, 2011.
- V. Balzani and F. Scandola, *Supramolecular Photochemistry*, Ellis Horwood, Chichester, 1991.
- D. W. Bruce and D. O'Hare, *Inorganic Materials*, John Wiley & Sons, New York, 1992.
- U. Schubert and N. Hüsing, *Synthesis of Inorganic Material*, Wiley-VCH, Weinheim, 2004.
- P. D. Yang, *The Chemistry of Nanostructured Materials*, World Scientific Publishing, Singapore, 2003.
- C. N. R. Rao, A. Muller and A. K. Cheetham, *The Chemistry of Nanomaterials: Synthesis Properties and Applications*, Wiley-VCH, Weinheim, Germany, 2004.
- G. Cao, *Nanostructures and Nanomaterials, Synthesis, Properties & Applications*, Imperial College Press, London, 2004. G. A. Ozin and A. C. Arsenault, *Nanochemistry: A Chemical Approach to Nanomaterials*, RSC Publishing, Cambridge, 2005.
- C. N. R. Rao, A. Muller and A. K. Cheetham, *Nanomaterials Chemistry: Recent Developments and New Directions*, Wiley-VCH, Weinheim, Germany, 2007.
- E. Ruiz-Hitzky, K. Ariga and Y. Lvov, *Bio-inorganic Hybrid Nanomaterials. Strategies, Syntheses, Characterization and Applications*, Wiley-VCH, Weinheim, 2008.
- A. Sayari and M. Jaroniec, *Nanoporous Materials*, World Scientific Publishing, Singapore, 2008.
- L. Cademartiri and G. A. Ozin, *Concepts of Nanochemistry*, Wiley-VCH, Weinheim, 2009.
- J. N. Lalena, D. A. Cleary, E. E. Carpenter and N. F. Dean, *Inorganic Materials Synthesis and Fabrication*, John Wiley & Sons, Inc. Hoboken, New Jersey, 2008.
- P. Comba, T. W. Hambley and B. Martin, *Molecular Modeling of Inorganic Compounds*, 3rd Edn, Wiley-VCH, Weinheim, 2009.
- S. R. Batten, S. M. Neville and D. R. Turner, *Coordination Polymers Design, Analysis and Application*, The Royal Society of Chemistry, Cambridge, 2009.
- M. -C. Hong and L. Chen (Eds), *Design and Construction of Coordination Polymers*, John Wiley & Sons, Inc, Hoboken, New Jersey, 2009.
- J. N. Lalena and D. A. Cleary, *Principles of Inorganic Materials Design*, 2nd Edn, John Wiley & Sons, Inc, Hoboken, New Jersey, 2010.
- V. Balzani, A. Credi and M. Venturi, *Molecular Devices and Machines*, Wiley-VCH, Weinheim, 2003.
- M. Petty, *Molecular Electronics: From Principles to Practice*, Wiley, Chichester, 2008.
- L. R. Macgillivray (Ed), *Metal-Organic Frameworks: Design and Application*, John Wiley & Sons, Inc, Hoboken, New Jersey, 2010.
- S. R. Marder, J. E. Sohn and G. D. Stucky (Eds), *Materials for Non-linear Optics: Chemical Perspectives*, ACS Symposium Ser, 1991.
- R. W. Boyd, *Nonlinear Optics*, Academic Press, San Diego, 1992.
- R.L. Carlin, *Magnetochemistry*, Springer-Verlag, New York, 1986. O. Kahn, *Molecular Magnetism*, VCH, New York, 1993.

- P. Day and A. E. Underhill (Eds), *Metal-organic and Organic Molecular Magnets*, RSC, London, 2000.
- P. M. Lathi (Ed), *Magnetic Properties of Organic Materials*, Marcel Dekker, New York, 1999.
- J. S. Miller and M. Drillon (Eds), *Magnetism: Molecules to Materials, V; Molecule-based Magnets*, Wiley-VCH, Weinheim, 2005.
- P. Gutlich and H. A. Goodwin, *Spin Crossover in Transition Metal Compounds I*, Springer, Berlin, 2004.
- F. E. Mabbs and D. J. Machin, *Magnetism and Transition Metal Complexes*, Dover Publications, 2008.
- R. Winpenny (Ed), *Single-Molecule Magnets and Related Phenomena*, Structure and Bonding Series, Vol. 122, Springer, Berlin, 2010.
- B. D. Cullity and C. D. Graham, *Introduction to Magnetic Materials*, 2nd Edn, John Wiley & Sons, New York, 2011.
- K. H. J. Buschow, *Handbook of Magnetic materials*, Vol 20, Elsevier, New York, 2012.
- D. Gatteschi, R Sessoli and J. Villain, *Molecular Nanomagnets*, Oxford University Press, Oxford, 2006.
- R. Hilzinger and W. Rodewald, *Magnetic Materials*, Wiley, New York, 2013.
- C. M. Sorensen, *Magnetism in Nanoscale Materials in Chemistry*, Wiley Interscience, New York, 2001.
- B. Pignataro (Ed), *Tomorrow's Chemistry Today – Concepts in Nanoscience, Organic Materials and Environmental Chemistry*, Wiley-VCH, Weinheim, 2008.
- L. Cademartiri and G. A. Ozin, *Concepts of Nanochemistry*, Wiley-VCH, Weinheim, 2008.
- B. R. Eggins, *Chemical Sensors and Biosensors*, Wiley India Pvt Ltd, New Delhi, 2002.
- S. Chandrasekhar, *Liquid Crystals*, 2nd Edn, Cambridge University Press, Cambridge, 1992.
- G. R. Desiraju, *Crystal Engineering: Designing of Organic Solids*, Elsevier, New York, 1989.
- D. Braga, F. Grepioni and A. G. Orpen, *Crystal Engineering: from Molecules and Crystals to Materials*, Kluwer Academic Publishers, Dordrecht, 1999.
- U. Schubert and N. Husing, *Synthesis of Inorganic Material*, 2nd Edn, Wiley-VCH Verlag GmbH & Co, Weinheim, 2005.
- X. -D. Xiang and I. Takenchi (Eds), *Combinatorial Synthesis*, Marcel Dekker, New York, 2003.
- E. I. Stiefel (Ed), *Dithiolene Chemistry: Synthesis, properties, and Applications*, John Wiley & Sons, New Jersey, 2004.
- P. Gomez-Romero and C. Sanchez (Eds), *Functional Hybrid Materials*, Wiley-VCH, Weinheim, 2004.
- R. S. Drago, *Physical Methods for Chemists*, Saunders, Philadelphia, 1993.
- M. F. C. Ladd and R. A. Palmer, *Structural Determination by X-ray Crystallography*, 3rd Edn, Plenum, New York, 1994.
- D. Farrusseng (Ed), *Metal-Organic Framework: Applications from Catalysis to Gas Storage*, Wiley-VCH, Verlag, GmbH & Co, 2011.

MSCH404-N: Nuclear-Analytical Major-III**Full Marks: 50, Credit: 4****1. Spectroscopy and Instrumentation**

Introduction, types of spectrometers, dispersive-, filter-based spectrometers, signal-to-noise ratio, principles of interferometer operation, quantitative explanation; parts of spectrophotometer, spectrofluorimeter, FT-IR, AAS, Mass, XRD, SEM, TEM.

2. Application of molecular spectroscopy in chemical analysis

Spectroscopic methods for trace and ultra-trace analysis: atomic absorption, flame photometry, atomic emission - theory, instrumentation and application, Raman spectroscopy - Raman effect, spectra and applications, photochemistry - laws, quantum yield - problems, instrumentation, photochemical reactions, actinometer, molecular luminescence- theory, instrumentation, application, effect of temperature and solvent effects in fluorescence

3. Application of mass spectroscopy in chemical analysis

Instrumentation, generation of ions, fragmentations and detection: EI, CI, FAB, ESI, MALDI, MALDI-TOF, etc. Electron Probe Micro-Analysis (EPMA), Laser Micro-Probe Mass Analyser (LAMMA) and Atomic Mass Spectrometry (AMS): theory, working principle and applications

4. Hyphenated techniques

State of the art, introduction on GC, LC, HPLC, criterion of hyphenation and its purpose, scope of versatility of hyphenated techniques: GC-MS, LC-MS, GC-FTIR, GC-MS-FTIR, GC-AED, LC-FTIR, LC-NMR -principle, application, limitation

5. Kinetic methods of analysis

Introduction, transition state theory, dielectric effect and ion-ion interaction, study of fast reaction, stopped flow, relaxation method, reaction involving structural changes and enzymatic processes; template reaction; self-exchange reaction, electron tunneling hypothesis, Marcus theory: inner-sphere and outer-sphere reaction, indicator reactions, application of kinetic methods in trace analysis

Recommended Books

- R. J. H. Clark and R. E. Hester, *Advances in Infrared and Raman Spectroscopy*, John Wiley, 1985.
 D. Rendell and D. Mowthrope, *Fluorescence and Phosphorescence Spectroscopy*, John Wiley, 1987.
 E. Metcalfe and F. E. Prichard, *Atomic Absorption and Emission Spectroscopy*, John Wiley, 1987.
 P. W. J. M. Boumans, *Inductively Coupled Plasma Emission Spectroscopy*, John Wiley, 1987.
 K. E. Jarvis, A. L. Gray and R. S. Houlik, *Hand Book of Inductively Coupled Plasma Emission Spectroscopy*, Blackie, Classgow and London, 1992.

D. J. Peters, J. H. Hayes and G.M. Hieftje, *Chemical Separation and Measurements*, Saunders, Philadelphia, 1974.

A. Welz, *Atomic Absorption Spectrometry*, Verlag, Weinheim, 1985.

W. Salvin, *Graphite Furnace AAS: A Source Book*, Perkin-Elmer, Norwalk, 1984.

G. W. Ewing, *Instrumental Methods of Chemical Analysis*, 4th Edn, McGraw Hill, 1978.

E. Y. Wehry, *Modern Fluorescence Spectroscopy*, Plenum Publishing Company, 1981

K. Nakamoto, *Infrared and Raman Spectroscopy of Inorganic and Coordination Compounds*, Wiley, 1986.

H. M. Kingston and L. B. Jassie (Ed), *Introduction to Microwave Sample Preparation: Theory and Practice*, American Chemical Society, Washington DC, 1988.

S. M. Khopkar, *Basic Concepts of Analytical Chemistry*, New Age International Ltd. Publishers, New Delhi, 1998.

D. A. Skoog, d. M. West and F. J. Holler, *Fundamentals of Analytical Chemistry*, 7th Edn, Saunders, Philadelphia, 1996.

- R. Kellner, J. M. Mermet, M. Otto and H. M. Widmer (Eds), *Analytical Chemistry*, Wiley-VCH, Weinheim, 1998.
- J. D. Ingel, Jr and S. R. Crouch, *Spectroscopic Analysis*, Prentice Hall, New Jersey, 1988.
- I. M. Kolthoff, P. J. Elving and E. B. Sandell, *Treatise on Analytical Chemistry*, Pt-I, II, III, The Interscience Encyclopedia, Inc., New York, 1959.
- A. I. Vogel, *A Test Book of Quantitative Inorganic Analysis*, 3rd Edn, Longmans, 1961.
- D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill, New York, 2000.
- D. A. Skoog, *Principle of Instrumental Analysis*, 3rd Edn, Saunders College Publishing, New York, 1985.
- D. A. Skoog and J. J. Leory, *Principles of Instrumental Analysis*, Saunders, Philadelphia, 1994.
- G. D. Christian, *Analytical Chemistry*, 5th Edn, John Wiley, New York, 1994.
- P. Tundo, A. V Perosa and F Zecchimi (Eds), *Methods and Reagents for Green Chemistry: An Introduction*, Wiley Interscience, New Jersey, 2007.
- R. K. Sharma, I. T. Sidhwami and M. K. Chaudhury, *Green Chemistry experiments: A Monograph*, Tucker Prakashan, New Delhi, 2007.
- R.Sanghi and M. M. Srivastava, *Green Chemistry, Environment Friendly Alternatives*, Narosa, New Delhi, 2008.
- R.Sanghi and V. Singh, *Green Chemistry for environmental remediation*, Wiley, New York, 2012.
- V. D. Scott and G. Love (Eds), *The Development of Electron-Probe Micro-Analysis—An Historical Perspective*, in *Quantitative Electron-Probe Microanalysis*, John Wiley & Sons Ltd, 1983.
- E. de Hoffmann and V. Stroobant, *Mass Spectrometry: Principles and Applications*, 2nd Edn, John Wiley & Sons Ltd, 2007.
- J. T. Watson and O. D. Sparkman, *Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation*, 4th Edn, John Wiley & Sons Ltd, 2007.
- J. Lovric, *Introducing Proteomics: From Concepts to Sample Separation, Mass Spectrometry and Data Analysis*, Wiley-Blackwell, 2011.

MSCH404-O: Organic Major-III

Full Marks: 50, Credit: 4

1. Pericyclic reactions II

Symmetry properties of MOs, orbital symmetry conservation and Woodward-Hoffmann rule in pericyclic reaction; frontier orbital interaction, Fukui-Hoffman theory (qualitative), Dewar theory of aromatic transition state concept (qualitative)

Definition, classification, electrocyclic reaction and the electroreversion reactions; sigmatropic reactions of [i,j] and [j,j] types; regioselectivity, stereoselectivity and stereospecificity in electrocyclic reactions; chelotropic reaction

2. Asymmetric synthesis

The chiral pool: synthesis and application; asymmetric Diels-Alder reaction and Heck reaction. Resolution –kinetic

3. Green chemistry II

Synthesis and applications of ionic liquids towards organic syntheses; organic reactions using supported reagents; solvent-free organic reactions; ultrasound and micro-wave assisted organic syntheses; real world cases of green chemistry

4. Baldwin's rules

Favored and disfavored ring-closure reactions

5. Steroids

Nomenclature of steroids and sterols, conformation, reactions and synthesis of steroids, cholesterol, Bile acids, steroid hormones, oestrogen, diosgenin, hecogenin, biosynthesis of sterols

6. Nucleic acids

Introduction, classification and occurrences of nucleosides; biosynthesis of α -D-ribose phosphate, inosinic acid, adenylic acid and guanylic acid, RNA and DNA (double helix structure with H-bonding)

7. Organo-main-group chemistry: sulfur, silicon and tin

Sulfur-stabilized anions: Sulfonium salts, Sulfonium and Sulfoxonium ylids, Sulfur-stabilized cations: The Pummerer rearrangement, Chiral sulfoxides in synthesis

Nucleophilic substitution at silicon; Silyl ethers; Alkynyl silanes; Aryl silanes; Vinyl silanes; Allyl silanes, Organotin compounds

Recommended Books

R. Streitwieser, *Molecular Orbital Theory of Organic Chemists*, John Wiley, New York, 1961.

R. B. Woodward and R. Hoffman, *The Conservation of Orbital Symmetry*, Verlag Chemie GmbH, 1970.

E. R. Lehr and A. P. Merchand, *Orbital Symmetry and Cyclo-addition*, Academic Press, New York, 1972.

G. B. Gills and M. R. Willis, *Pericyclic Reactions*, Chapman and Hall, London, 1974.

A. H. Depuy and O. H. Chapman, *Molecular Reaction and Organic Photochemistry*, Prentice-Hall, New York, 1975.

- T. L. Gilchrist and R. C. Storr, *Organic Reactions and Orbital Symmetry*, 2nd Edn, Cambridge University Press, Cambridge, 1979.
- I. Fleming, *Frontier Orbitals and Organic Chemical Reactions*, John Wiley, New York, 1980.
- R. O. C. Norman and J. M. Coxon, *Principles of Organic Synthesis*, 3rd Edn, ELBS, London, 2003.
- R. E. Ireland, *Organic Synthesis*, Prentice-Hall, New York, 1969.
- R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley, New York, 1994.
- W. Caruthers, *Modern Methods of Organic Synthesis*, 3rd Edn, Cambridge University Press, Cambridge, 1996.
- T. H. Lowry and K. C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3rd Edn, Harper and Row, New York, 1998.
- F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry, Parts A and B*, 4th Edn, Plenum Press, New York, 2001.
- P. T. Anastas and J. C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, USA, 2000.
- R. Sanghi, M. M. Srivastava, *Green Chemistry*, Narosa Publishing House, India, 2003.
- R. K. Sharma, I. T. Sidhwani, M. K. Chaudhuri, *Green Chemistry Experiments: A Monograph*, Tucker Prakashan, India, 2007.
- H. W. Roesky, D.K. Kennepohl, *Experiments in Green and Sustainable Chemistry*, Wiley-VCH, Weinheim, 2009.
- M. Lancaster, *Green Chemistry: An Introductory Text*, 2nd Edn, Royal Society of Chemistry, UK, 2010.
- V. K. Ahluwalia, *Strategies for Green Organic Synthesis*, CRC Press, Boca Raton, FL, 2012.
- L. F. Fieser and M. Fieser, *Steroids*, Reinhold, New York, 1967.
- J. S. Bindra and R. Bindra, *Prostaglandin Synthesis*, Academic Press, New York, 1983.
- L. J. Goad and T. Akisha, *Analysis of Sterols*, Blackie Academic and Professional, 1997.
- R. L. Pecsok, L. D. Shields, T. Cairns and I. G. McWilliam, *Modern Methods of Chemical Analysis*, 2nd Edn, 1996.
- A. Mazur and B. Harrow, *Text Book of Biochemistry*, 10th Edn, W.B. Saunders Co, 1971.
- T. M. Devlin, *Text Book of Biochemistry*, 2nd Edn, John Wiley, New York, 1986.
- P. W. Kuchel and G. B. Ralston, *Theory and Problems in Biochemistry*, International Edn, McGraw-Hill, 1988.
- G. Thomas, *Medicinal Chemistry – An Introduction*, John Wiley, New York, 2001.
- J. M. Berg, J. L. Tymoczko and L. Stryer, *Biochemistry*, 5th Edn, W.H. Freeman Co, 2002.
- D. L. Nelson and M. M. Cox, *Lehninger: Principle of Biochemistry*, 4th Edn, W. H. Freeman Co, 2005.

MSCH404-P: Physical Major-III**Full Marks: 50, Credit: 4**

1. Approximate methods in quantum mechanics

Principles of linear and non-linear variation methods, stationary perturbation theory for non-degenerate and degenerate states - applications to rotator, Stark effect, the He-atom; Time dependent perturbation theory, semiclassical treatment of radiation-matter interaction, transition probability and rates, Einstein's A and B coefficients, selection rules

2. Quantum Chemistry III

Angular momentum: operators, their commutation properties, step-up and step-down operators, application to single electron and multi-electron atom, eigen-ket-ladder and formulation of spherical harmonics from angular momentum rules, finite rotation operation vs. angular momentum operators, spin angular momentum, Pauli spin matrices — spin eigenfunctions and their properties

3. Quantum Chemistry IV

Antisymmetry of many electron wave function, spin and spatial orbitals, Slater determinant; closed-shell and open-shell electron configurations; multi-electron pure-spin state wave functions - examples with 2- and 3-electron systems, formulation of a multi-electron closed-shell electron configuration energy, introduction of core, Coulomb and exchange integrals with their properties - example of He atom, independent particle model, multi-electron atomic Hartree Hamiltonian and related SCF equations solution, vertical ionization potential and Koopman's theorem; variational solution of the closed-shell wave function - formulation of the Hartree-Fock equations, properties of Hartree-Fock operator and wave functions, discussion of electron correlation

Recommended Books

L. Pauling and E. B. Wilson, *Introduction to Quantum Mechanics*, McGraw-Hill, New York, 1939.

H. Eyring, J. Walter and G. F. Kimball, *Quantum Chemistry*, Wiley, New York, 1944.

J. L. Powell and B. Crasemann, *Quantum Mechanics*, Addison-Wesley, 1961.

E. Merzbacher, *Quantum Mechanics*, John Wiley & Sons, New York, 1970.

L. I. Schiff, *Quantum Mechanics*, McGraw-Hill, New York, 1985.

S P. C. W. Davies, *Quantum Mechanics*, ELBS, London, 1985.

A. K. Chandra, *Introductory Quantum Chemistry*, Tata McGraw-Hill Publishing Co, New Delhi, 1989.

F. L. Pilar, *Elementary Quantum Chemistry*, Tata McGraw-Hill, New Delhi, 1990.

D. Bohm, *Quantum Theory*, Asia Pub House, 1960.

P. W. Atkins, *Molecular Quantum Mechanics*, Clarendon Press, Oxford, 1980.

R. McWeeny, *Methods of Molecular Quantum Mechanics*, Academic Press, London, 1989.

D. A. McQuarrie, *Quantum Chemistry*, Viva Books Pvt Ltd, New Delhi, 2003.

G. C. Schatz and M. A. Ratner, *Quantum Mechanics in Chemistry*, Dover Publication, Inc, New York, 2002.

H. L. Strauss, *Quantum Mechanics*, Eastern Economy Edition, Prentice Hall of India Pvt. Ltd., New Delhi.

Practical papers

MSCH405-I Inorganic Major-II Practical Full Marks: 50 Credit: 4

1. Preparation of inorganic and coordination compounds and their characterization
 - a. Elemental Analysis (C,H,N and S, AAS or other analytical methods)
 - b. Growing of single crystals and their X-ray diffraction studies
 - c. Spectral, thermal, electrochemical and magnetic studies
2. Kinetic and mechanistic studies of some selected reactions (substitution and redox)

MSCH405-N Nuclear Analytical Major-II Practical Full Marks: 50, Credit: 4

1. Experiments with GM detector: Dead time calculation and calibration with multi-channel analyser
2. Use of γ -ray spectrophotometer
3. Some γ radio-analytical experiments

MSCH405-O Organic Major-II Practical Full Marks: 50, Credit: 4

1. Preparation of organic compounds involving multiple step reactions
2. Characterization of organic compounds

MSCH405-P Physical Major-II Practical Full Marks: 50, Credit: 4

1. Instrumental methods of studying hydrolysis, solubility and kinetics; elementary computer-based numerical methods
2. Study on charge transfer/EDA complexes

MSCH406-I Inorganic Project/Term Paper Full Marks: 50, Credit: 4

Topic selection in consultation with the teacher; literature search from different reference books and using internet search; typed write-up with proper tables, structures, figures and literature to be submitted (approximately 25-30 pages with 12 font size); seminar lecture on this topic to be delivered in presence of all the teachers and an external subject expert

MSCH406-N Nuclear-Analytical Project/Term Paper Full Marks: 50, Credit: 4

Topic selection in consultation with the teacher; literature search from different reference books and using internet search; typed write-up with proper tables, structures, figures and literature to be submitted (approximately 25-30 pages with 12 font size); seminar lecture on this topic to be delivered in presence of all the teachers and an external subject expert

MSCH406-O Organic Project/Term Paper Full Marks: 50, Credit: 4

Topic selection in consultation with the teacher; literature search from different reference books and using internet search; typed write-up with proper tables, structures, figures and literature to be submitted (approximately 25-30 pages with 12 font size); seminar lecture on this topic to be delivered in presence of all the teachers and an external subject expert

MSCH406-P Physical Project/Term Paper Full Marks: 50, Credit: 4

Topic selection in consultation with the teacher; literature search from different reference books and using internet search; typed write-up with proper tables, structures, figures and literature to be submitted (approximately 25-30 pages with 12 font size); seminar lecture on this topic to be delivered in presence of all the teachers and an external subject expert.
