

**DRAFT SYLLABUS**

For

M. Sc. Course in

Chemistry

To be effective from the session 2014-15



**THE UNIVERSITY OF BURDWAN**

**BURDWAN 713 104**

**WEST BENGAL, INDIA**

## THE UNIVERSITY OF BURDWAN

## Syllabus for M. Sc. Course in Chemistry

## Course Structure

S E M E S T E R  I	Paper	Core Subject	Marks <sup>*</sup>	Credit <sup>**</sup>
	MCHEM0101	Inorganic General I	50	4
	MCHEM0102	Nuclear-Analytical General I	50	4
	MCHEM0103	Organic General I	50	4
	MCHEM0104	Physical General I	50	4
		<b>Practical Papers</b>		
	MCHEM0105	Inorganic General Practical	50	3.75
	MCHEM0106	Nuclear-Analytical General Practical	50	3.75
		<b>Total</b>	<b>300</b>	<b>23.5</b>

S E M E S T E R  II	Paper	Core Subject	Marks <sup>*</sup>	Credit <sup>**</sup>
	MCHEM0201	Inorganic General II	50	4
	MCHEM0202	Nuclear-Analytical General II	50	4
	MCHEM0203	Organic General II	50	4
	MCHEM0204	Physical General II	50	4
		<b>Practical Papers</b>		
	MCHEM0205	Organic General Practical	50	3.75
	MCHEM0206	Physical General Practical	50	3.75
		<b>Total</b>	<b>300</b>	<b>23.5</b>

S E M E S T E R  III	Paper	Core Subject	Marks <sup>*</sup>	Credit <sup>**</sup>
	MCHEM0301	Advanced Inorganic General	50	4
	MCHEM0302	Advanced Nuclear-Analytical General	50	4
	MCHEM0303	Advanced Organic General	50	4
		<b>Major Electives (any one)</b>		
	MCHEM0304	Inorganic Major I	50	4
	MCHEM0305	Nuclear-Analytical Major I	50	4
	MCHEM0306	Organic Major I	50	4
	MCHEM0307	Physical Major I	50	4
		<b>Practical Papers (MCHEM 0308 and any one from MCHEM 0309-0312)</b>		
	MCHEM0308	Computer Applications in Chemistry General	50	3.75
	MCHEM0309	Inorganic Major Practical I	50	3.75
	MCHEM0310	Nuclear-Analytical Major Practical I	50	3.75
	MCHEM0311	Organic Major Practical I	50	3.75
	MCHEM0312	Physical Major Practical I	50	3.75
		<b>Total</b>	<b>300</b>	<b>23.5</b>

S E M E S T E R  IV	Paper	Core Subject	Marks <sup>*</sup>	Credit <sup>**</sup>
	MCHEM0401	Advanced Physical General	50	4
		<b>Major Electives (any one from MCHEM 0402-0405 and any one from MCHEM 0406-0409)</b>		
	MCHEM0402	Inorganic Major II	50	4
	MCHEM0403	Nuclear-Analytical Major II	50	4
	MCHEM0404	Organic Major II	50	4
	MCHEM0405	Physical Major II	50	4
	MCHEM0406	Inorganic Major III	50	4
	MCHEM0407	Nuclear-Analytical Major III	50	4
	MCHEM0408	Organic Major III	50	4
	MCHEM0409	Physical Major III	50	4
		<b>Major Elective Practical (any one)</b>		
	MCHEM0410	Inorganic Major Practical II	50	3.75
	MCHEM0411	Nuclear-Analytical Major Practical II	50	3.75
	MCHEM0412	Organic Major Practical II	50	3.75
	MCHEM0413	Physical Major Practical II	50	3.75
		<b>Term Paper/Project<sup>#</sup> (any one from MCHEM 0414-0417 and MCHEM 0418 is common to all)</b>		
	MCHEM0414	Inorganic Term Paper/Project	40	3.75
	MCHEM0415	Nuclear-Analytical Term Paper/Project	40	3.75
	MCHEM0416	Organic Term Paper/Project	40	3.75
	MCHEM0417	Physical Term Paper/Project	40	3.75
	MCHEM0418	Social Outreach	10	1
		<b>Minor Elective Subjects<sup>##</sup> (CBC) (any one of the following two)</b>		
	MCHEM0419	Industrial Chemistry	50	2
	MCHEM0420	Environmental Chemistry	50	2
		<b>Total</b>	<b>300</b>	<b>22.5</b>
		<b>Grand Total</b>	<b>1200</b>	<b>93.0</b>

\* Marks: Sem I + Sem II + Sem III + Sem IV = 300 + 300 + 300 + 300 = 1200;

\*\*Credits: Sem I + Sem II + Sem III + Sem IV = 23.5 + 23.5 + 23.5 + 22.5 = 93.0;

<sup>#</sup>For term paper/project: preparation + presentation + viva-voce = 20 + 10 + 10 = 40;

<sup>##</sup>Number of students intake for minor electives will depend on the availability of seats.

**Semester-I (Total Marks 300, Credit 23.5)****Theoretical****MCHEM 0101: Inorganic General I****Marks: 50, Credit: 4****1. Bonding and properties in chemical systems – a quantum chemical approach**

Preamble, LCAO and/or Huckel treatments of sigma- and pi-MOs (inorganic di- and polyatomic species and organic units like alkanes, alkenes, allyl system, dienes, polyenes – open and cyclic, sandwich molecules, boron compounds, etc.) with a closer look into the orbital symmetry, molecular term symbols, relative energy, transition probability, selection rules, nature and intensity of transitions (allowed/forbidden), probing reaction centre, and aromaticity of inorganic, organic, coordination and organometallic species; Koopmans' theorem, Walsh diagram, isolobal analogy

**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

**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≡C bonds, hydride and dihydrogen complexes, phosphines and related ligands, spectral analysis and characterization, Dewar-Chat-Duncanson bonding model, isolobal analogy, Agostic interaction

**4. Bioinorganic and inorganic medicinal chemistry**

Background, myoglobin, hemoglobin, hemocyanin, hemerythrin, cytochromes, rubredoxin, ferredoxins; biological nitrogen fixation, chlorophyll and photosynthesis; PS-I, PS-II, bioenergetics and ATP cycle, glucose storage, Na<sup>+</sup>/K<sup>+</sup> ion pump, ionophores, metalloenzyme – catalase, peroxidase, ceruloplasmin, cytochrome oxidase, carbonic anhydrase, carboxy peptidase, metallothionein, xanthine oxidase, sulphite oxidase, nitrate reductase, superoxide dismutase, chemistry of respiration; vitamin B<sub>12</sub> and B<sub>12</sub>-enzyme

Metals in medicines: diseases due to deficiencies, carcinogenesis, applications of chelators and metal chelates of different generations; antitumour, anticancer and anti-AIDS drugs, mechanistic pathway, limitation

***Tentative List of 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, *Coulson's Valence*, 3<sup>rd</sup> 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*, 2<sup>nd</sup> 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*, 3<sup>rd</sup> Edn, John Wiley & Sons, New York, 1999.
- F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6<sup>th</sup> Edn, John Wiley & Sons, Inc, New York, 1999.
- B. Douglas, D. McDaniel and J. Alexander, *Concepts and Models of Inorganic Chemistry*, 3<sup>rd</sup> 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*, 4<sup>th</sup> Edn, Pearson, New Delhi, 2006.
- D. A. McQuarrie, P. A. Rock and E. B. Gallogly, *General Chemistry*, 4<sup>th</sup> Edn, University Science Books, Mill Valley, Canada, 2011.
- 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*, 2<sup>nd</sup> 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*, 4<sup>th</sup> 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*, 2<sup>nd</sup> Edn, Chapman and Hall, London, 1988.
- J. D. Atwood, *Inorganic and Organometallic Reaction Mechanisms*, 2<sup>nd</sup> Edn, VCH, New York, 1997.
- R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 4<sup>th</sup> Edn, Wiley, New York, 2005.
- C. Elschenbroich, *Organometallics*, 3<sup>rd</sup> 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 2<sup>nd</sup> 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. Lipperd and J. S. Valentine, *Bioinorganic Chemistry*, Viva Books Pvt. Ltd., New Delhi, 1998.
- A. Das and G. N. Mukherjee, *Elements of Bioinorganic Chemistry*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> Edn, Elsevier, New York, 2012.
- R. M. Roat-Malone, *Bioinorganic Chemistry: A short Course*, 2<sup>nd</sup> Edn, Wiley, New York, 2013.
- G. Patrick, *Instant Notes: Medicinal Chemistry*, Viva Books, New Delhi, 2002.
- G. L. Patrik, *An Introduction to Medicinal Chemistry*, 3<sup>rd</sup> Edn, Oxford University Press, 2006.
- A. Kar, *Medicinal Chemistry*, 4<sup>th</sup> 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.

#### MCHEM 0102: Nuclear-Analytical General I

Marks: 50, Credit: 4

##### 1. Nuclear properties and structure I

Fundamentals, Rutherford's experiments, nuclear composition and qualitative idea of different nuclear forces; mass-energy relationship, nuclear binding energy and its role in nuclear stability, concept of nuclear angular momentum, magnetic dipole moment and electronic quadrupole moment (elementary idea), 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 semiempirical 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: TGA, DTA, DSC; thermogram, applications, thermal stability of covalent and non-covalent bonds, thermal degradation, single crystal phase transformation, thermochemiluminescence, different types of titrations and their applications, solid state reaction kinetics

## 6. Green chemistry and environmental chemistry

Sustainable development, twelve principles of green chemistry and implementations, atom economy, environmental E-factor, role of catalysts, microwave and ultrasound irradiation in green synthesis, traditional and alternative commercial syntheses of ibuprofen, adipic acid and maleic acid etc, green chemistry in action developing foam, whitening agent, detergent builders, green insecticides, biosynthesis of synthetic chemical, photochemical reactions in atmosphere, photochemical smog and stratospheric ozone depletion; chemicals from renewable feedstocks

### ***Tentative List of 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*, 3<sup>rd</sup> Edn, Jhon Wiley & Sons Inc, New York, 1981.
- H. J. Arnikaar, *Essentials of Nuclear Chemistry*, 4<sup>th</sup> 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 Zecchini (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*, 4<sup>th</sup> Edn, New Age International (P) Ltd Publications, New Delhi, 2000.

**MCHEM 0103: Organic General I****Marks: 50, Credit: 4****1. Conformation and reactivity of acyclic and cyclic systems**

Acyclic compounds: The Felkin Anh model, The Howk model and Sharpless asymmetric epoxidation; cyclic compounds: monocyclic (3- to 8-membered rings) and bicyclic compounds (bridged, fused and spiro)

**2. Structure-reactivity relationship: A quantitative approach**

Linear free energy relations: Hammett equation, Hammett's  $\sigma_x$  and  $\rho$  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 the following compounds and their derivatives: imidazole, pyrazole, oxazole, isoxazole, thiazole and iso-thiazole and triazole systems

**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. Polymerization**

Monomer, dimer, dendrimer and polymer; mechanism of formation: carbonyl substitution reactions, electrophilic aromatic substitution, the  $S_N2$  reaction and nucleophilic attack on isocyanates; polymerization of alkenes; co-polymerization; biodegradable polymers and plastics; reactions on polymers

***Tentative List of Recommended Books***

- D. Nasipuri, *Stereochemistry of Organic Compounds*, 2<sup>nd</sup> 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*, 4<sup>th</sup> 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*, 6<sup>th</sup> Edn, Pearson Education Ltd, New Delhi, 2011.
- R. Kartritzky, *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*, 4<sup>th</sup> Edn, New Age International (P) Ltd, India, 2005.
- J. A. Joule, K. Mills, *Heterocyclic Chemistry*, 5<sup>th</sup> 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*, 3<sup>rd</sup> 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*, 4<sup>th</sup> Edn, Wiley Interscience, New Jersey, 2004.
- P. C. Hiemenz and T. P. Lodge, *Polymer Chemistry*, 2<sup>nd</sup> Edn, CRC Press, Boca Raton, FL, 2007.



## 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

Overview of experimental findings; identification of classical and quantum systems, Bohr's correspondence principle, postulates of quantum mechanics, properties of wave functions, operators and related theorems; degeneracy, spread of observation and uncertainty principle

## 3. Elementary 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 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 in terms of partition function

## 5. Atomic spectra

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: classification of molecules into spherical, symmetric and asymmetric tops; diatomic molecules as rigid rotors - energy levels, selection rules and spectral features, isotope effect, intensity distribution, effect of non-rigidity on spectral features; vibrational spectra of diatomics: 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 of diatomics, resonance Raman spectroscopy; NMR spectra: theory, relaxation process, spin interactions - its origin, equivalent protons, qualitative idea of energy levels of AX, AX<sub>2</sub> and AX<sub>3</sub> systems, a few representative examples

***Tentative List of 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. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3<sup>rd</sup> 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*, 3<sup>rd</sup> 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*, 4<sup>th</sup> 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.

### Practical

#### MCHEM 0105: Inorganic General Practical

Marks: 50, Credit: 3.75

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

#### MCHEM 0106: Nuclear-Analytical General Practical

Marks: 50, Credit: 3.75

1. Separation techniques involving ion exchange and solvent extraction
2. Titrimetric estimation of different organic compounds
3. Beer's law: application in different chemical matrices

**Semester-II (Total Marks 300, Credit 23.5)****Theoretical****MCHEM 0201: Inorganic General II****Marks: 50, Credit: 4****1. Chemistry of elements and their compounds**

Elements – structural versatility and related properties; compounds – design, benign, modular and reticular 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

Mono- and polynuclear compounds of lanthanoid and actinoid ions stressing on choice of different multidentate chelators and congregators with special emphasis on electric, magnetic, conducting, superconducting and fluorophoric behaviours

**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, chevreton 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.

***Tentative List of 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*, 2<sup>nd</sup> Edn, Pergamon, New York, 1997.

F. A. Cotton, G. Wilkinson, C. M. Murillo and M. Bochmann, *Advanced Inorganic Chemistry*, 6<sup>th</sup> 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*, 3<sup>rd</sup> Edn, John Wiley & Sons, Inc, New York, 2001.

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

- J. E. Huheey, E. A. Keiter, R. L. Keiter and O. K. Medhi, *Inorganic Chemistry: Principles of Structures and Reactivity*, 4<sup>th</sup> 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*, 3<sup>rd</sup> 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, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> Edn, John Wiley and Sons, New York, 2009.
- P. Powell, *Principles of Organometallic Chemistry*, 2<sup>nd</sup> 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 2<sup>nd</sup> 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.
- M. H. Chisholm (Ed), *Early Transition Metal Clusters with  $\pi$ -Donor Ligands*, VCH, New York, 1995.
- 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*, 3<sup>rd</sup> Edn, Pearson Education Ltd, Essex, England, 2008.
- A. F. Wells, *Structural Inorganic Chemistry*, 5<sup>th</sup> 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*, John Wiley & 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*, 4<sup>th</sup> Edn, CRC Press, Boca Raton, FL, 2012.
- A. R. West, *Solid State Chemistry and Its Application*, 2<sup>nd</sup> Edn, Wiley-VCH, Weinheim, 2014.

## MCHEM 0202: 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 superheavy elements, separation chemistry

### 4. Separation techniques

Preamble, successive extraction and separation; techniques of solvent extraction: Craig extraction and counter current distribution; ionic liquid assisted and supercritical solvent extraction, problems; chromatography: mathematical relations of capacity, selectivity factor, distribution constant and retention time; chromatogram, elution in column chromatography: band broadening and column efficiency; van Deemter equation; column resolution, numerical problems, gas chromatography, high performance chromatography and supercritical fluid chromatography: principles, methods, comparison and applications; size-exclusion chromatography, ion chromatography and 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

### ***Tentative List of 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*, 3<sup>rd</sup> Edn, John Wiley & Sons Inc., New York, 1981.
- G. Seaborg, *Modern Alchemy*, World Scientific, Singapore, 1994.

- H. J. Arnikar, *Essentials of Nuclear Chemistry*, 4<sup>th</sup> 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*, 5<sup>th</sup> 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*, 5<sup>th</sup> 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*, 2<sup>nd</sup> Edn, Wiley, New York, 1998.
- C. G. Zoski (Ed) *Handbook of Electrochemistry*, Elsevier, New York, 2007.

## MCHEM 0203: 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

Abnormal mutarotation of monosaccharides; use of complexing agents: borates, phosphates and copper compound; synthesis of glycosides; general treatment of polysaccharide chemistry: isolation, purification, hydrolysis, methylation and periodic oxidation, Smith degradation, Barry degradation

### 3. Spectroscopy

Ultraviolet

Transitions, vacuum ultraviolet, rules of Eglinton & Meakins: applications in conjugated dienes, trienes, polyenes, Woodward's rules for enones and its application in  $\alpha,\beta$ -unsaturated carbonyl compounds; solvent effect, applications in aromatic and heterocyclic compounds

#### Infrared

Fundamentals, stretching and bending vibrations, application identification of functional groups, applications in sequence of organic synthetic reactions and in the structure elucidation of organic molecules, FTIR

#### $^1\text{H}$ -NMR

Nuclear spin states and magnetic moments, chemical shift, shielding and deshielding, origin of spin-spin coupling, Pascal's triangle, tree-diagrams, coupling constant and its measurement, germinal and vicinal couplings, Karplus equation, homoallylic and allylic couplings, First-order and Non-first-order spectra, Pople notation, chemical exchange, chemical shift reagents, NOE, structure elucidation

#### 4. Mass Spectrometry

Electron impact mass spectroscopy, low and high resolution, exact masses of nucleides, molecular ions, isotope ions, mass marking techniques, fragment ions of odd and even electron types, rearrangement ions, factors affecting cleavage patterns

#### ***Tentative List of Recommended Books***

- J. March, *Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, 5<sup>th</sup> 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*, 4<sup>th</sup> 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*, 3<sup>rd</sup> Edn, Harper and Row, New York, 1998.
- I. L. Finar, *Organic Chemistry*, Vol I, 6<sup>th</sup> Edn, Addison Wesley Longmann, London, 1998.
- I. L. Finar, *Organic Chemistry*, Vol II, 5<sup>th</sup> 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*, 3<sup>rd</sup> Edn, Clarendon Press, Oxford, 1988.
- J. Kennedy, *Carbohydrate Chemistry*, Clarendon Press, Oxford, 1988.
- R. T. Morison, and R. N. Boyd, *Organic Chemistry*, 6<sup>th</sup> Edn, Prentice-Hall India Pvt Ltd, New Delhi, 1992.
- J. R. Dyer, *Applications of Absorption Spectroscopy of Organic compounds*, 2<sup>nd</sup> 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*, 3<sup>rd</sup> Edn, McMillan, Hong Kong, 1991.
- R. M. Silverstein and F. Webster, *Spectrometric Identification of Organic Compounds*, 6<sup>th</sup> Edn, John Wiley, New York, 1998.

- D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 5<sup>th</sup> 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*, 2<sup>nd</sup> 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.

## MCHEM 0204: 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 and construction of their character tables, direct product representations, projection operators (without derivations) and vanishing of integrals, invariance of the Hamiltonian operator and eigenfunctions of H as bases of irreducible representations

### 2. Quantum mechanics II

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

### 3. Electrochemistry

Introduction, ion-solvent interaction: Born model and Born equation, enthalpy of ion-solvent interaction and its calculation, Eley-Evan model, solvation number and methods for determination of solvation number, ion association: Bjerrum equation, fraction of ions associated, ion association constant; electrode kinetics: relation between current and rate of electrode reaction, current-overpotential relationship, Tafel equation and its importance

### 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, Curtin-Hammett principle, linear free energy relationship, Hammett and Taft equation; study of fast reactions — flow process and relaxation techniques

### 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.



***Tentative List of 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. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3<sup>rd</sup> 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*, 3<sup>rd</sup> Edn, Narosa Publishing House, New Delhi, 1995.
- R. A. Alberty and R. J. Silbey, *Physical Chemistry*, 1<sup>st</sup> 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*, 4<sup>th</sup> 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*, 3<sup>rd</sup> Edn, Plenum Press, New York, 1994.
- X. Clegg, *Crystal Structure Determination*, Oxford University Press, Oxford, 2005.

**Practical****MCHEM 0205: Organic General****Marks: 50, Credit: 3.75**

1. Separation of binary mixtures of solid-solid/liquid-solid/liquid-liquid organic compounds and identification of individual components
2. Synthesis of organic compounds involving important chemical reactions (nitration, diazotisation, Beckmann transformation, photochemical reaction, Sandmeyer reaction, pinacol-pinacolone rearrangement)

**MCHEM 0206: Physical General****Marks: 50, Credit: 3.75**

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 23.5)****Theoretical****MCHEM 0301: 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

## 3. Application of surfactants

Preamble, classification of surfactants, micellisation, synthetic application of micellar catalysis, mixed micelles, foaming of surfactant solution, different types of interface, emulsion and emulsifier, photochemistry and redox reaction in micellar systems, nanoemulsion and stabilisation

## 4. Atomic spectrometry in inorganic analysis

General remark, instrumentation and application; electrothermal atomization, cold vapour and hydride generation techniques and theories involved; atomic absorption, atomic emission, atomic fluorescence and inductively-coupled plasma AES

## 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 I

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

***Tentative List of 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 6<sup>th</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 1<sup>st</sup> Edn, John Wiley & Sons, Chichester, 2012.

### MCHEM 0302: Advanced Nuclear-Analytical General

Marks: 50, Credit: 4

#### 1. Complexes in aqueous solution

pH-potentiometric, spectrophotometric methods (slope-ratio, mole-ratio and Job's method of continuous variation) of measuring stability constants of complexes, Bjerrum half n method, stability of mixed ligand complexes and calculations; determination of composition, evaluation of thermodynamic parameters, factors influencing the stability of complexes

#### 2 Advanced spectroscopic methods:

Instrumentation, presentation of spectra, Applications of heteronuclear NMR spectroscopy; <sup>11</sup>B, <sup>13</sup>C, <sup>14</sup>N, <sup>17</sup>O, <sup>19</sup>F and <sup>31</sup>P-NMR, <sup>195</sup>Pt. CD/ORD: methods, molecular dissymmetry and chiroptical properties, Cotton effect, Faraday effect in magnetic circular dichroism (MCD) and application. 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

## 6. Radiopharmaceuticals

Nuclear pharmacy: concept, pharmaceuticals and radiopharmaceuticals; radionuclide generators; ideal radiopharmaceuticals, methods of radiolabelling, specific radiopharmaceuticals for diagnostic and therapeutic purposes

### ***Tentative List of 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> Edn, Wiley, New York, 1998.

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

### MCHEM 0303: 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: rearrangement of unsaturated compounds; photo-induced reactions in aromatic compounds

#### 2. Pericyclic reaction I

Definition, classification, cyclo-additions and cyclo-reversion reactions, [2+2], [2+4], [4+6] reactions, catalysis; electrocyclic reaction and the electroreversion reactions; sigmatropic reactions of [i,j] and [j,j] types, regioselectivity, periselectivity in cycloadditions; generalised rules of pericyclic reactions

#### 3. Reaction with cyclic transition states or cyclic intermediates

Tethering, Robinson annulations, iodolactonisation; synthesis of transfused ring; sulfur as a tether

#### 4. Reagents in organic synthesis

Hydride transfer reagent: Boranes, trialkyl borohydrides, Diimide, Baker's yeast, trialkyl tin hydride; DIBAL, Na(CN)BH<sub>3</sub>, Woodward and Prevost hydroxylation, Sharpless epoxidation, PCC, PDC, Mn(IV) oxide, RuO<sub>4</sub> (TPAP), Moffat oxidation, Swern oxidation, Dess-Martin Periodinane; Shapiro reaction, Peterson reaction, OsO<sub>4</sub>, SeO<sub>2</sub>

#### 5. Medicinal chemistry

Drugs: introduction, classification of drugs, brief discussion of drug targets, antibiotics: penicillin, chloramphenicol etc., drug targets on nucleic acids, definition of antagonist, agonist, prodrugs, pharmacokinetics and pharmacodynamics, concept of structure-activity relationship (SAR) and quantitative structure and relationship (QSAR)

### ***Tentative List of 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*, 2<sup>nd</sup> 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*, 3<sup>rd</sup> Edn, Harper and Row, New York, 1998.

H. O. House, *Modern Synthetic Reactions*, 2<sup>nd</sup> Edn, Benjamin, 1971.

W. Caruthers, *Modern Methods of Organic Synthesis*, 3<sup>rd</sup> 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*, 3<sup>rd</sup> Edn, ELBS, 2003.
- J. Singh and J. Singh, *Photochemistry and Pericyclic Reactions*, 3<sup>rd</sup> Edn, New Age International (P) Ltd, India, 2012.
- A. Griesbeck, M. Oelgemoller and F. Ghetti, *Organic Photochemistry and Photobiology*, 3<sup>rd</sup> Edn, Vol I, CRC Press, Boca Raton, FL, 2012.
- F. D. King, *Medicinal Chemistry: Principles And Practice*, 2<sup>nd</sup> Edn, Royal Society of Chemistry, 2002.
- G. L. Patrick, *An Introduction to Medicinal Chemistry*, 3<sup>rd</sup> Edn, Oxford University Press Inc, New York, 2005.
- A. Kar, *Medicinal Chemistry*, 4<sup>th</sup> Edn, New Age International (P) Ltd, India, 2007.
- C. G. Wermuth, *The Practice of Medicinal Chemistry*, 3<sup>rd</sup> Edn, Academic Press, New York, 2008.

#### MCHEM 0304: Inorganic Major I

Marks: 50, Credit: 4

##### 1. Synthetic methodology for inorganic, coordination and organometallic compounds

Ligand design and ligand synthesis, tailoring and appending of pendant arm, ligand topology and molecular mechanics; coordination compound design and synthesis using classical and green methods, self-assembly, atom economy, thermolysis, photolysis, sonolysis, electrolysis, sol-gel method, hydrothermal method, cryochemistry, combinatorial chemistry, top-down and bottom-up methods for nano-structured solids, biomodeling

##### 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, metalloidligand, probing chemical reactivity and reaction pathways (intramolecular/intermolecular, stereoretentivity/stereodynamicity), covalency of ML bonding and comment on bonding theories

#### ***Tentative List of 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*, 6<sup>th</sup> 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*, 4<sup>th</sup> 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*, 3<sup>rd</sup> Edn, Wiley-VCH, Weinheim, 2008.
- J. W. Steed and J. L. Atwood, *Supramolecular Chemistry*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> Edn, VCH, Weinheim, 1991.
- R. H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 2<sup>nd</sup> 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*, 4<sup>th</sup> Edn, Wiley, New York, 2005.
- D. Steinborn, *Fundamentals of Organometallic Catalysis*, John Wiley & Sons, New York, 2011.
- G. Aruldas, *Molecular Structure and Spectroscopy*, 2<sup>nd</sup> 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, 6<sup>th</sup> 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. Cradock, *Structural Methods in Inorganic Chemistry*, 2<sup>nd</sup> 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.

### MCHEM 0305: Nuclear-Analytical Major I

**Marks: 50, credit: 4**

#### 1. Theory of radioactive decay

Introduction, quantum mechanical aspects of radioactive disintegration, alpha decay paradox and its explanation in terms of tunnel effect, Geiger-Muller relationship, time-dependant perturbation theory, Golden rule and its application in explaining beta and gamma transition, selection rules

#### 2. Nuclear force and structures

Two body problem - properties of deuteron and derivation of depth-range relationship, its applications in explaining nature of nuclear force, elementary particles; nuclear models - strong and weak interaction, nuclear magnetic dipole moment and electric quadruple moment in terms of shell model, collective model, Fermi gas model, nuclear excitation, idea of nuclear temperature and entropy

#### 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

#### 4. Nuclear detectors

Classification of nuclear detectors, variation of amplitude vs. voltage - characterization of different zones, G. M. detector -operational principle dead time -role of quench gases - limitations and applications, proportional detectors: proportional counter performance, flow-type proportional counter, gas multiplication factor, space charge effects, resolution, time characteristics of signal pulse; scintillation detectors: different types with examples, pulse shape analysis, resolution and detection efficiency, liquid scintillation detectors; detection of neutrons, semiconductor detector: general characterization, depletion depth, reverse bias, requirement of cryogenic condition, resolution and efficiency, pulse rise

time, with a brief account of n-type and p-type semiconductor, Si lattice, Ge-Li, Si-Li - a comparison intrinsic and doped-semiconductor-fabrication surface barrier detector; some basic ideas of pulse processing and shaping, single- and multi-channel analysers, digital and analogue systems, applications in space research, development of detector assembly with requirement of newer space and defence technology viz., nuclear missile

#### 5. Coincidence counting

Determination of absolute disintegration rates, decay scheme studies

#### ***Tentative List of 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*, 2<sup>nd</sup> 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*, 4<sup>th</sup> 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, 4<sup>th</sup> Edn, New Delhi, 2001.

#### **MCHEM 0306: 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 carophyllene, abietic acid,  $\beta$ -amyrin,  $\alpha$  and  $\beta$ -carotenoids

3.  $^{13}\text{C}$  NMR spectroscopy

Introduction, theory, instrumentation, chemical shifts, coupling constants, proton-decoupled, off-resonance-decoupled  $^{13}\text{C}$  NMR spectrum, NOE effect, DEPT experiment, application in structure elucidation of organic compounds

## 4. Stereo selective reactions of alkenes and carbonyl compounds

Nucleophilic addition: use of chiral substrates, auxiliaries, reagents and catalysts; asymmetric conjugate addition; addition of allyl boron derivative; reactions at alpha carbon: enolate formation (regioselectivity and stereoselectivity); stereoselective enolate alkylation (oxazolidinone, oxazoline); aldol reaction, asymmetric aldol reaction; hydrogenation, dihydroxylation, cyclopropanation, epoxidation

## 5. ORD-CD

Introduction, theory, Cotton effect curves and applications, octant rule, axial halo ketone rule, lactone sector rule

***Tentative List of 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*, 2<sup>nd</sup> Edn, John Wiley, New York, 1994.
- R. C. Mehrotra and A. Singh, *Organometallic Chemistry : A Unified Approach*, 2<sup>nd</sup> 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. Hanessian, *Total Synthesis of Natural Products: The Chiron Approach*, Pergamon Press, Oxford, 1984.
- I. L. Finar, *Organic Chemistry*, Vol II, 5<sup>th</sup> 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,  $^{13}\text{C}$  NMR Spectroscopy : Methods and Application in Organic Chemistry, 3<sup>rd</sup> 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*, 3<sup>rd</sup> Edn, Cambridge University Press, Cambridge, 1996.
- T. H. Lowry and K. C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3<sup>rd</sup> Edn, Harper and Row, New York, 1998.
- J. March, *Advanced Organic Chemistry: Reactions, Mechanism and Structure*, 5<sup>th</sup> Edn, John Wiley, New York, 1999.
- F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry, Parts A and B*, 4<sup>th</sup> 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*, 3<sup>rd</sup> 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*, 2<sup>nd</sup> 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.

### MCHEM 0307: 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 force, 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. Applications of group theory

Construction of SALC's and their use in calculation of  $\pi$  MO's under the Huckel approximations, (ii) calculation of MO's 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

Production of excited states, singlet and triplet states, radiative and non-radiative processes, fluorescence and phosphorescence: mirror image relationship, quantum yield and life-time; phenomenological approach of quenching,

transient effects; properties of excited states: dipole moment,  $pK_a$ , energy transfer, photoinduced electron transfer, excimers and exciplexes; special photochemical reactions, flash photolysis, laser flash photolysis

### ***Tentative List of 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*, 5<sup>th</sup> 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* 1<sup>st</sup> 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. Vincent, *Molecular Symmetry and Group Theory*, John Wiley & Sons, New York, 1998.
- F. A. Cotton, *Chemical Applications of Group Theory*, 3<sup>rd</sup> 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. Birks, *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**

**MCHEM 0308: Computer Application in Chemistry General**

**Marks: 50, Credit: 3.75**

#### **A. Theoretical**

##### **1. Introduction to computers**

Scope for computers, present-day position, computer overview and organization; hardware: CPU, memory – volatile and non-volatile, I/O devices and controllers; software: concept of stored programmes, information storage and retrieval, control instructions and data, idea of operating system, driver and controller programmes, utility packages, user programmes and code.

##### **2. Number system**

Decimal, binary, octal and hexadecimal representations, negative numbers and floating point numbers, character sets (ASCII, EBCDIC), fixed and floating point arithmetic

**3. Introduction to DOS and WINDOWS**

Concept of file, record, data, bit, byte, block; track, sector on storage media; use of file editors — EDIT, NORTON, word Processors etc.

Data types, arithmetic operations and expressions, relational expressions, library functions, I/O and format statements, control statements, nesting of loops, block IF, subroutines and function subprograms, subscribed variables, dimension and common, parameter passing between programme modules, file handling (OPEN, CLOSE, INQUIRE, REWIND, BACKSPACE, ENDFILE)

**4. Numerical techniques and chemical applications**

Algorithms, logical analysis of problems, flow-chart, programmes, data fitting by least square, interpolation techniques, iterative methods, solution of simultaneous equations

**5. Elements of C language****B. Practical**

On-hand practical training with computers on selected chemical problems

***Tentative List of Recommended Books***

S. Lipschutz, A. Poe, *Programming with FORTAN* (Schaum Series), Mc-Graw-Hill International Edition, Singapore, 1982.

V. Rajaraman, *Computer programming in FORTAN IV*, PHI, New Delhi, 1982.

B. W. Kernighan, D. M. Ritchie, *The C programming Language*, PHI, Eastern Economy Edition, New Delhi, 1996.

V. Rajaraman, *Computer programming in C*, PHI, New Delhi, 1996.

R. S. Salaria, *Numerical Methods*, B. P. B. Publications, New Delhi, 1996.

S. D. Conte and C. de Boor, *Elementary Numerical Analysis*, McGraw-Hill International, New Delhi, 1986.

E. G. Lewars, *Computational Chemistry: Introduction to the Theory and Applications of Molecular and Quantum Mechanics*, Springer (India) Pvt Ltd, 2007.

**MCHEM 0309: Inorganic Major Practical I****Marks: 50, Credit: 3.75**

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. Determination of composition and formation constants of selected systems by pH-metric and spectrophotometric methods

**MCHEM 0310: Nuclear-Analytical Major Practical I****Marks: 50, Credit: 3.75**

1. Quantitative analysis of major, minor and trace components of ores and alloys by conventional and instrumental methods like spectrophotometer and AAS
2. Analysis of water, cement, fertilizer, food and drug

**MCHEM 0311: Organic Major Practical I**  
**Credit, 3.75**

**Marks: 50,**

1. Different types of chromatographic techniques
2. Quantitative estimation of organic compounds
3. Isolation of selected natural products: Caffeine from Tea, Casein and Lactose from milk etc

**MCHEM 0312: Physical Major Practical I**

**Marks: 50, Credit: 3.75**

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

**Semester-IV (Total Marks 300, Credit 22.5**

**Theoretical**

**MCHEM 0401: Advanced Physical General**

**Marks: 50, Credit: 4**

1. Diffraction study

Diffraction of X-Ray by crystal, Laue and Bragg condition, concept of reciprocal lattice, crystal structure factor, systematic absence, techniques in X-Ray structure determination

2. Surface chemistry

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

3. Macromolecules

Introduction; Carothers' equation, average molecular weights & their determination; 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

4. Non-ideal systems

Virial equations, second Virial coefficient; 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

5. Quantum chemistry

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; Laguerre and associated Laguerre polynomials; polynomials as orthonormal functions, their properties; complete solution of the H-atom problem; 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

## 6. Spectroscopy

Maxwell's field equations, transition between states, selection rules and forbidden transitions; NMR: Relaxation and exchange phenomena, theories of chemical shift and nuclear spin-spin coupling in 2-spin systems with applications, pulsed NMR (spin echo); Electronic:  $n \rightarrow \pi^*$ ,  $\pi \rightarrow \pi^*$  and CT transitions; vibrational: simple polyatomic molecules, normal modes, influence of nuclear spin on vibration-rotation spectra of polyatomics

***Tentative List of Recommended Books***

- R. C. Evans, *An Introduction to Crystal Chemistry*, 2<sup>nd</sup> Edn, Cambridge University Press, Cambridge, 1964.
- M. F. C. Ladd and R. A. Palmer, *Structural Determination by X-ray Crystallography*, 3<sup>rd</sup> 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*, 2<sup>nd</sup> 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*, 3<sup>rd</sup> Edn, Narosa Publishing House, 1995.
- R. A. Alberty and R. J. Silbey, *Physical Chemistry*, 1<sup>st</sup> Edn, John Wiley and Sons, Inc, New York, 1995.
- I. N. Levine, *Physical Chemistry*, 4<sup>th</sup> 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*, 4<sup>th</sup> 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.

## MCHEM 0402: Inorganic Major II

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, quasireversible and irreversible electrochemical and chemical processes in model compounds; electro-induced reactions: protic/electroprotic equilibrium, electrocatalysis, electropolymerisation, electrocrystallisation, electrochemiluminescence; electrosynthesis, evaluating comproportionation constant, OTTLE, surface-modified electrode, photoelectrochemistry, spectroelectrochemistry, 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

### *Tentative List of 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*, 2<sup>nd</sup> 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*, 5<sup>th</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> Edn, Arnold, London, 1997.
- C. H. Hamann, A. Hammett and W. Vielstich, *Electrochemistry*, Wiley-VCH, New York, 1998.
- A. J. Bard and L. F. Faulkner, *Electrochemical Methods – Fundamentals and Applications*, 2<sup>nd</sup> Edn, Wiley, New York, 1998.
- G. E. Marcelle, *Molten Salts: From Fundamentals to Applications*, Kluwer Academic Publisher, 2001.
- C. H. Hamann, A. Hammett 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*, 4<sup>th</sup> Edn, Oxford, 2006.
- G. L. Miessler and D. A. Tarr, *Inorganic Chemistry*, 3<sup>rd</sup> 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. Mowthorpe, *Fluorescence and Phosphorescence Spectroscopy*, John Wiley, New York, 1987.
- C. E. Wayne and R. P. Wayne, *Photochemistry*, Oxford University Press, 1<sup>st</sup> Indian Edn, New Delhi, 2005.
- J. R. Lakowicz, *Principles of fluorescence spectroscopy*, 3<sup>rd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> Edn, Wiley-VCH, Weinheim, 1997.
- S. Asperger, *Chemical Kinetics and Inorganic Reaction Mechanisms*, 2<sup>nd</sup> Edn, Springer, London, 2012.

### **MCHEM 0403: Nuclear-Analytical Major II**

**Marks: 50, Credit: 4**

#### **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,  $K_0$  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 programme right from Homi Bhaba, requirement of more nuclear energy in Indian scenario neglecting and justifying controversies.

General features and 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 particular reference to glass

#### ***Tentative List of 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*, 3<sup>rd</sup> 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.

#### **MCHEM 0404: Organic Major II**

**Marks: 50, Credit: 4**

##### 1. Organic photochemistry II

Photo-induced functionalisation in organic molecules involving Barton reaction, Hofmann-Löffler-Freytag reaction; photochemical rearrangements, photo induced disproportion reaction, photo induced substitution reaction in aromatic systems, chemiluminescence in organic 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. Any advanced topic

##### 5. Organic synthetic process

Retrosynthetic analysis; C-C bond formation reactions; synthesis of L-hexose (Sharpless and Masamune), prostaglandins, Crixivan, etc

##### 6. Spectroscopy and stereochemistry

NMR;  $^3J$  variation with dihedral angle, fused rings, spreading out effect, vicinal coupling in other ring sizes, geminal coupling; shapes of NMR signals, pi contribution, 2D-NMR, EI-MS, MALDI-TOF-MS

7. Any advanced topic

### ***Tentative List of 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*, 3<sup>rd</sup> Revised Edn, New Age International (P) Ltd, New Delhi, 2012.
- A. Griesbeck, M. Oelgemoller and F. Ghatti, *Organic Photochemistry and Photobiology*, 3<sup>rd</sup> 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*, 5<sup>th</sup> 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*, 3<sup>rd</sup> 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*, 3<sup>rd</sup> Edn, McMillan, Hong Kong, 1991.
- D. H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 5<sup>th</sup> Edn, Tata McGraw-Hill, New Delhi, 2005.
- R. M. Silverstein and F. Webster, *Spectrometric Identification of Organic Compounds*, 6<sup>th</sup> 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.

### MCHEM 0405: Physical Major II

**Marks: 50, Credit: 4**

#### 1. Statistical 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 and theorem, microcanonical, canonical and grand canonical 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

#### 2. 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, Curie law

#### 3. Molecular interactions

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

#### ***Tentative List Recommended of 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*,

## 1. Supramolecular chemistry II

Geometry setter, blocker, spacer and their judicious choice, hydrogen bonding, pi-pi, C-H...pi, halogen...pi, S...pi, etc interactions, allosterism, proton and hydride sponges, principle of three C's, lock and key principle, host-guest interaction, self organization and self complementarity, receptors, superstructures in inorganic, metallo-organic and organometallic compounds, 0D, 1D, 2D, 3D architectures and hierarchies, supramolecular devices

## 2. Inorganic materials

Molecules and crystals to materials, scaffold, art of synthesis, interwoven bonding, predictable crystalline architecture, intermolecular and interion interactions, secondary building unit (SBU), 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

## 4. Structure-function relationship

A sheer necessity and an ultimatum, thermodynamic and kinetic parameters; diagnostic probes: spectroscopic, thermal, electrochemical, magnetic, crystallographic; parameters: stretching frequency, chemical shift, spin-spin coupling constant, isomer shift, potential value, bond distance, bond angle, torsion angle, crystal packing and Madelung constant, magnetic moment value, rate constant, half life, correlation diagram, room temperature and variable-temperature results, breakthrough and legacy

***Tentative List of Recommended Books***

G. A. Jefferey 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. 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*, 1<sup>st</sup> 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*, 2<sup>nd</sup> 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*, 3<sup>rd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 2<sup>nd</sup> 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*, 3<sup>rd</sup> Edn, Plenum, New York, 1994.
- D. Farrusseng (Ed), *Metal-Organic Framework: Applications from Catalysis to Gas Storage*, Wiley-VCH, Verlag, GmbH & Co, 2011.

### MCHEM 0407: Nuclear-Analytical Major III

**Marks: 50, Credit: 4**

#### 1. Application of molecular spectroscopy in chemical analysis

Introduction to instrumental methods for trace and ultra-trace analysis: atomic absorption, flame photometry, atomic emission, atomic fluorescence - theory, instrumentation and application, Raman spectroscopy - Raman effect, applications, spectra of typical molecules, photochemistry - laws, quantum yield - problems, instrumentation, examples of

photochemical reactions, actinometer, molecular lumininescence spectrometry - theory, instrumentation, application, effect of temperature and solvent effects in fluorescence

## 2. Kinetic method 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

## 3. 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

## 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. Applied analysis

Sampling, modern methods of sample digestion, typical analysis of ores, minerals, alloys, glass and ceramic materials, fuel, food, food additives, drug, pesticides in fruit juice and water

## 6. Basic electronics

Characteristics and use of diodes, capacitors, inductors, transformers, FET, MOSFET, rectifier, power supply, clipper, oscillator and timer circuits, linear small signal amplifiers and their characteristics, integrated circuits, operational amplifier and its applications including applications in analytical and nuclear instruments, logic gates and elementary digital circuits

## 7. 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

### ***Tentative List of Recommended Books***

R. J. H. Clark and R. E. Hester, *Advances in Infrared and Raman Spectroscopy*, John Wiley, 1985.

D. Rendell and D. Mowthorpe, *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. Houk, *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*, 4<sup>th</sup> 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*, 7<sup>th</sup> 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*, 3<sup>rd</sup> Edn, Longmans, 1961.
- D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill, New York, 2000.
- D. A. Skoog, *Principle of Instrumental Analysis*, 3<sup>rd</sup> 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*, 5<sup>th</sup> 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*, 2<sup>nd</sup> Edn, John Wiley & Sons Ltd, 2007.
- J. T. Watson and O. D. Sparkman, *Introduction to Mass Spectrometry: Instrumentation, Applications, and Strategies for Data Interpretation*, 4<sup>th</sup> Edn, John Wiley & Sons Ltd, 2007.
- J. Lovric, *Introducing Proteomics: From Concepts to Sample Separation, Mass Spectrometry and Data Analysis*, Wiley-Blackwell, 2011.

### MCHEM 0408: Organic Major III

**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); dipolar cyclo-additions, chelotropic reaction, ene reactions, selection rules

#### 2. Asymmetric synthesis

The chiral pool: synthesis and application; asymmetric Diels-Alder reaction and Heck reaction

### 3. Green methodologies for organic synthesis

Twelve principles of green chemistry, green synthetic methods: green reagents; green solvents and reaction conditions; green catalysis; real world cases of green chemistry, organic reactions in aqueous medium, organic reactions using supported reagents, solvent-free organic reactions, micro-wave assisted organic reactions, use of ionic liquid, supercritical fluids

### 4. Any advanced topic

### 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  $\alpha$ -D-ribose phosphate, inosinic acid, adenylic acid and guanylic acid, RNA and DNA (double helix structure with H-bonding)

### 7. Organic Synthetic Methods

Chemistry of organo-boron, -sulfur, -silicon and -tin towards organic synthesis

### 8. Any advanced topic

### ***Tentative List of 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*, 2<sup>nd</sup> 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*, 3<sup>rd</sup> 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*, 3<sup>rd</sup> Edn, Cambridge University Press, Cambridge, 1996.
- T. H. Lowry and K. C. Richardson, *Mechanism and Theory in Organic Chemistry*, 3<sup>rd</sup> Edn, Harper and Row, New York, 1998.
- F. A. Carey and R. J. Sundberg, *Advanced Organic Chemistry, Parts A and B*, 4<sup>th</sup> 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, Weiheim, 2009.
- M. Lancaster, *Green Chemistry: An Introductory Text*, 2<sup>nd</sup> 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*, 10<sup>th</sup> Edn, W.B. Saunders Co, 1971.
- T. M. Devlin, *Text Book of Biochemistry*, 2<sup>nd</sup> 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*, 5<sup>th</sup> Edn, W.H. Freeman Co, 2002.
- D. L. Nelson and M. M. Cox, *Lehninger: Principle of Biochemistry*, 4<sup>th</sup> Edn, W. H. Freeman Co, 2005.

### MCHEM 0409: Physical Major III

**Marks: 50, Credit: 4**

#### 1. Analysis of quantum mechanical principles

Analysis of the postulates - pictures and representations; properties of sets of functions, Schmidt orthonormalisation; Fourier transformation, delta function with examples, free particle normalization; matrix formulation, tunneling, bound states, the Virial theorem

#### 2. Approximate methods in quantum mechanics

Time dependent perturbation theory, semiclassical treatment of radiation-matter interaction, transition probability and rates, Einstein's A and B coefficients, selection rules; 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

#### 3. Quantum Chemistry

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

### ***Tentative List of 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

#### MCHEM 0410: Inorganic Major Practical II

Marks: 50, Credit: 3.75

1. Preparation of inorganic and coordination compounds and their characterization
  - a. Bi-, tri- and polydentate ligands
  - b. Complexation and purification
  - c. Growing of single crystals
  - d. Elemental analyses (C, H, N and AAS)
  - e. Spectral, thermal, electrochemical and magnetic studies
  - f. Reactivities
2. Kinetic and mechanistic studies of some selected reactions (substitution and redox)

#### MCHEM 0411: Nuclear-Analytical Major Practical II

Marks: 50, Credit: 3.75

1. Experiments with GM detector: Dead time calculation and calibration with multi-channel analyser
2. Use of  $\gamma$ -ray spectrophotometer
3. Some radioanalytical experiments

#### MCHEM 0412: Organic Major Practical II

Marks: 50, Credit: 3.75

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

#### MCHEM 0413: Physical Major Practical II

Marks: 50, Credit: 3.75

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

**MCHEM 0414: Inorganic Term Paper/Project****Marks: 40, Credit: 3.75**

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

**MCHEM 0415: Nuclear-Analytical Term Paper/Project****Marks: 40, Credit: 3.75**

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

**MCHEM 0416: Organic Term Paper/Project****Marks: 40, Credit: 3.75**

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

**MCHEM 0417: Physical Term Paper/Project****Marks: 40, Credit: 3.75**

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

**MCHEM 0418: Social Outreach****Marks: 10, Credit: 1**

Students will be asked to take part in different social awareness programmes, decided by the department time to time

**MCHEM 0419: Industrial Chemistry****Marks: 50, Credit: 2**

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

Portland cement: Manufacture, characteristics, setting of cement, testing

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

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

Nanochemistry: Preparation and Properties of Nanomaterials; Some Special Nanomaterials like Carbon Nanotubes and Fullerenes; Applications in different fields.

Corrosion and prevention: Corrosion in iron and steel industries, chemical industries, building, different forms of prevention of corrosion in different industries.

**MCHEM 0420: Environmental Chemistry****Marks: 50, Credit: 2**

Elements of environment, pollution and pollutants, biodiversity, sustainable ecosystem

Air pollution: primary pollutants ( $\text{CO}_2$ ,  $\text{NO}_2$ ,  $\text{SO}_2$ , HCs, VOCs), photochemical smog, SPM, greenhouse effect, ozone hole and generation of ozone in the atmosphere, El Nino

Water pollution: organic and inorganic pollutants, radioactive materials, thermal pollutants; Ground water pollution/arsenic contamination, waste water treatment, water quality

Soil pollution: waste classification and disposal, solid waste management, detoxification of toxic wastes; radioactive pollution, noise pollution and health

Energy resources: conventional and non-conventional energy sources, sustainable development

Environmental management: Sectoral examples- thermal power plants, bioparks, chemical industries, textile industries, tanneries, food processing industry, aquaculture projects