

# **CURRICULUM OF CHEMISTRY**

**MSc Program  
(2-Year, 4-Semester)**



**Department of Chemistry**  
Shaheed Benazir Bhutto Women University  
Peshawar

# **SCHEME OF STUDIES**

**(Session 2016 onward)**

## MSc (2-year, 4-Semester)

### Scheme of Studies

<u>First Semester</u>		<u>Second Semester</u>	
<u>Course Code</u>	<u>Credits</u>	<u>Course Code</u>	<u>Credits</u>
CH-321	2 + 1	CH-322	2 + 1
CH-331	2 + 1	CH-332	2 + 1
CH-341	3 + 1	CH-342	3 + 1
CH-351	3 + 1	CH-352	3 + 1
CH-050	2 + 0	CH-301	2 + 0
Total:	<hr/> 16 <hr/>	Total:	<hr/> 16 <hr/>

<u>Third Semester</u>	<u>Credits</u>
Three theory courses of 2 credits each. Two theory courses of 3 credits each.	Theory 12
One practical course/Thesis of 3 credits.	Practical 3
One theory course (compulsory) of 3 credits for all specializations	Theory 3
Total:	<hr/> 18 <hr/>

<u>Fourth Semester</u>	<u>Credits</u>
Three theory courses of 2 credits each. Two theory courses of 3 credits each.	Theory 12
One practical course/Thesis of 3 credits.	Practical 3
Total:	<hr/> 15 <hr/>

#### Compulsory Course:

Two theory courses (Functional English-I/II) of 2 credits each in the first two semesters (I-II).

**Total Credit Hours: 69**

## M.Sc. Courses (Chemistry)

### I. Analytical/Inorganic Chemistry

CH-321	Analytical Chemistry-I (Cr. 2 + 1)
CH-331	Inorganic Chemistry-I (Cr. 2 + 1)
CH-301	Industrial Chemistry (Cr. 2)
CH-322	Analytical Chemistry-II (Cr. 2 + 1)
CH-332	Inorganic Chemistry-II (Cr. 2 + 1)
CH-421	Principles and Applications of Molecular Spectrophotometry (Cr. 3)
CH-422	Atomic Spectroscopy (Cr. 3)
CH-423	Advanced Analytical Chemistry (Cr. 2)
CH-427	Crystallography (Cr. 3)
CH-428	Organometallic Chemistry (Cr. 2)
CH-429	Bio-coordination Chemistry (Cr. 2)
CH-430	Elementary Group Theory (Cr. 2)
CH-431	Coordination Chemistry (Cr. 3)
CH-432	Inorganic Chemistry-III (Cr. 2)
CH-433	Inorganic Chemistry-IV (Cr. 2)
CH-434	Inorganic Polymers (Cr. 2)
CH-435	Thesis/Research Project in Inorganic/Analytical Chemistry (Cr. 3)
CH-436	Nuclear and Radiochemistry (Cr. 2)
CH-437	Inorganic/Analytical Chemistry Laboratory-III (Cr. 3)
CH-438	Thesis/Research Project in Inorganic/Analytical Chemistry (Cr. 3)
CH-439	Advanced Inorganic/Analytical Chemistry Laboratory-IV (Cr. 3)

### II. Organic Chemistry

CH-341	Organic Chemistry-I (Cr. 3 + 1)
CH-342	Organic Chemistry-II (Cr. 3 + 1)
CH-440	Chemistry of Heterocycles (Cr. 2)
CH-441	Reaction Mechanism (Cr. 3)
CH-442	Spectroscopic Methods in Organic Chemistry-I (Cr. 2)
CH-443	Chemistry of Natural Products (Cr. 3)
CH-444	Reaction Mechanism-II (Cr. 3)
CH-445	Stereochemistry (Cr. 3)
CH-446	Retrosynthesis (Cr. 3)
CH-447	Organic Chemistry Laboratory-III (Cr. 3)
CH-448	Thesis/Research Project in Organic Chemistry (Cr. 3)
CH-449	Advanced Organic Chemistry Laboratory-IV (Cr. 3)
CH-470	Biochemistry (Cr. 2)
CH-471	Name Reactions (Cr. 2)
CH-472	Introduction to Polymer Chemistry (Cr. 3)
CH-473	Quantum Organic Chemistry (Cr. 2)
CH-474	Spectroscopic Methods in Organic Chemistry-II (Cr. 3)
CH-475	Thesis/Research Project in Organic Chemistry (Cr. 3)

### III. Physical Chemistry

CH-050	Basic Mathematics for Chemistry (Cr. 2)
CH-351	Physical Chemistry-I (Cr. 3 + 1)
CH-352	Physical Chemistry-II (Cr. 3 + 1)
CH-450	Computational Chemistry (Cr. 2)
CH-451	Chemical Kinetics (Cr. 3)
CH-452	Quantum Chemistry (Cr. 3)
CH-453	Molecular Spectroscopy (Cr. 3)
CH-454	Chemical Thermodynamics (Cr. 3)
CH-455	Statistical Mechanics (Cr. 2)
CH-456	Nuclear and Radiation Chemistry (Cr.2)
CH-457	Solid State Chemistry (Cr. 2)
CH-458	Solution Chemistry (Cr. 2)
CH-459	Physical Chemistry Laboratory-III (Cr. 3)
CH-460	Thesis/Research Project in Physical Chemistry (Cr. 3)
CH-461	Advanced Physical Chemistry Laboratory-IV (Cr. 3)
CH-462	Electrochemistry (Cr. 2)
CH-463	Polymer Chemistry (Cr. 2)
CH-464	Surface Chemistry (Cr. 2)
CH-465	Photochemistry (Cr.2)
CH-466	Colloids and Surfactants (Cr. 2)
CH-467	Thesis/Research Project in Physical Chemistry (Cr. 3)

#### **Compulsory Course for all specializations (3<sup>rd</sup> Semester)**

CH-360	Environmental Chemistry (Cr. 3)
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## Details of M.Sc. Courses (Chemistry)

### I. Analytical/Inorganic Chemistry

#### 1<sup>st</sup> Semester

##### CH-321 Analytical Chemistry-I (Cr. 2)

**Introduction:** Importance, application, growth of analytical chemistry. **Analytical Sampling:** Analytical data, data handling, statistical treatment of data. **Stoichiometry:** Stoichiometric calculations, chemical reactions. Concept of mole. **Chemical Equilibrium:** Law of mass action, degree of dissociations, theoretical principles, acid-base equilibria, solubility equilibria, complexation equilibria. **Quantitative Analytical Methods:** Potentiometry, conductometry, instrumentation, application.

##### **Recommended Books**

1. G.D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley & Sons Ltd., Singapore (2003).
2. D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill Companies Inc. (2000).
3. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, *Fundamentals of Analytical Chemistry*, 8<sup>th</sup> ed., Thomson Books/Cole, Belmont, USA (2004).

##### **Supplementary Books**

1. D.C. Harris, *Quantitative Chemical Analysis*, 5<sup>th</sup> ed., W.H. Freeman Company, New York (1999).
2. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2<sup>nd</sup> ed., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).
3. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Analysis*, 6<sup>th</sup> ed., Pearson Education Ltd. (2000).
4. R.B. Fischer, D.C. Peters, *Basic theory and concepts of Quantitative Chemical Analysis*, W.B. Saunders Company (1986).

##### CH-321 Analytical Chemistry Lab-I (Cr. 1)

*Note:- Out of thirteen any ten experiments would be conducted.*

1. To determine the exact weights of materials and to analyze replicate measurements statistically.
2. To calibrate volumetric apparatus and to investigate errors in delivered volume.
3. To determine the concentration of a strong acid solution by conductometric titration.

- To determine the individual concentration of the acids in the given binary mixture of a strong/weak acid conductometrically.
- To evaluate  $K_{sp}$  for lead iodate by conductance method.
- To determine solubility product of cadmium iodate titrimetrically.
- To establish the constancy of the solubility product.
- To estimate  $Ca^{2+}$  and  $Mg^{2+}$  concentration in drinking water by EDTA complexometric titration method.
- To determine concentration of a strong acid potentiometrically using first and second derivative methods.
- To determine  $pK_a$  for the given set of weak acids by the potentiometric method.
- To show independence of solubility on amount of undissolved species.
- To establish the stoichiometric relation for the precipitation of silver chloride.
- To prepare a buffer solution and study its buffering capacity.

#### **Recommended Books**

- G.D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley & Sons Ltd., Singapore (2003).
- R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2<sup>nd</sup> ed., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).

#### **CH-331 Inorganic Chemistry-I (Cr. 2)**

**Periodic table:** Periodic classification and periodic properties of the elements. **Theories of bonding:** Chemical bonding – valence bond and molecular orbital theories; shapes of inorganic molecules – VSEPR theory. **Theories of acids and bases:** Bronsted Lowry, solvent systems definition, Lewis acid-base concept, hard soft acids and basis. **Zero-group elements:** Their isolation, properties and uses. **Interhalogen compounds:** Chemistry of interhalogens, pseudohalogens and polyhalides.

#### **Recommended Books**

- F.A. Cotton, et al., *Advanced Inorganic Chemistry*, 6<sup>th</sup> ed., John Wiley, New York (1999).
- J.E. Huheey, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> ed., Addison-Wesley, Reading (1993).
- M.C. Day Jr. and Jod Selbin, *Theoretical Inorganic Chemistry* by Reinhold Publishing Corporation, New York (1962).

### Supplementary Books

1. A.J. Emeleus and A.G. Sharp, *Modern Aspects of Inorganic Chemistry*, Read K. Paul, London (1983).
2. T. Moeller, *The Chemistry of the Lanthanides*, Chapman and Hall Ltd. London (1965).
3. J.D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall London (1996).

### CH-331 Inorganic Chemistry Laboratory-I (Cr. 1)

Separation of metal ions by paper chromatography, estimation of pair of metal ions like  $\text{Cu}^{2+}/\text{Ni}^{2+}$ ,  $\text{Al}^{3+}/\text{Fe}^{3+}$ ,  $\text{Ca}^{2+}/\text{Ba}^{2+}$ ,  $\text{Zn}^{2+}/\text{Pb}^{2+}$ , estimation of halide ions.

### Recommended Book

1. A.I. Vogel, *A Textbook of Quantitative Inorganic Analysis: Theory and Practice*, Green and Co. Ltd., London (2000).

### 2<sup>nd</sup> Semester

Note:- Following course CH-301 is mandatory for all students of 2<sup>nd</sup> semester.

### CH-301 Industrial Chemistry (Cr. 2)

**Industrial units:** Basic data for the development of the industrial unit e.g. basic chemical data, chemical control, raw materials etc. Chemical processes i.e. unit operations, unit process. **Chemistry and technology of industries:** Water conditioning, cement, glass, ceramic, leather, fertilizers, sugar and starch, oil, fats and waxes, soap and detergent, pulp and paper etc.

### Recommended Books

1. D.D.L. Chung, *Composite Materials: Functional Material of Modern Technologies*, Springer-Verlag, London (2003).
2. F.L. Mathews and R.D. Rawlings, *Composite Materials: Engineering and Science*, Chapman and Hall, London (1994).
3. T.L. Vigo and B.J. Kinzig, *Composite Applications: The role of Matrix, Fiber and Interface*, VCH, New York (1992).

### CH-322 Analytical Chemistry-II (Cr. 2)

**Spectrometry:** Basic concepts, classification, theoretical concepts. **UV/visible spectrophotometry:** Introduction, Lambert-Beer Law, deviations, applications. **Solvent Extraction:** Distribution coefficient, distribution ratio, percent extraction, solvent extraction of metal complexes. **Chromatography:** Principles and theory, types of chromatography, paper chromatography, thin layer chromatography, column and gas chromatography. **Electrogravimetry:** Theory and principles, instrumentation, separation of metal ions, applications. **Voltammetry:** Introduction, instrumentation and applications of voltammetry and polarography.



### **Recommended Books**

1. D.C. Harris, *Quantitative Chemical Analysis*, 5<sup>th</sup> ed., W.H. Freeman Company, New York (1999).
2. D.A. Skoog and J.J. Leary, *Principles of Instrumental Analysis*, 4<sup>th</sup> ed., Saunders College Publishing, USA (1992).
3. H.H. Willard, L.L. Merritt, J.A. Dean, F.A. Settle, *Instrumental Methods of Analysis*, Wiley, New York (2003).

### **Supplementary Books**

1. G.D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley & Sons Ltd., Singapore (2003).
2. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, *Fundamentals of Analytical Chemistry*, 8<sup>th</sup> ed., Thomson Books/Cole, Belmont, USA (2004).
3. D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill Companies Inc. (2000).
4. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2<sup>nd</sup> ed., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).
5. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Analysis*, 6<sup>th</sup> ed., Pearson Education Ltd. (2000).
6. R. de Levie, *Principles of Quantitative Chemical Analysis*, McGraw-Hill Companies, Inc. (1997).

### **CH-322 Analytical Chemistry Lab-II (Cr. 1)**

#### ***Electrogravimetry:***

- To determine Copper(II) in solution by electrogravimetric method.
- To separate and quantify copper in brass using constant-current electrolysis.

#### ***Spectrophotometry:***

- To estimate Nickel(II) in solution spectrophotometrically.
- Spectrophotometric determination of ammonia.
- To determine Iron(II) by spectrophotometric method using o-phenanthroline.
- Colorimetric determination of Iron(III) with potassium thiocyanate.
- To verify Beer's law and to evaluate molar extinction coefficient.

### ***Chromatography:***

- To separate Fe(III), Co(II), Ni(II) and Cu(II) from solution using paper chromatography.

### ***Distribution Coefficient:***

- To determine distribution coefficient of a given solute between an aqueous/non-aqueous system.

### ***Amperometry:***

- To estimate lead amperometrically through titration with potassium dichromate.

### ***Titrimetry:***

- To determine Calcium by the indirect titration with EDTA.
- To determine Zinc by direct titration with EDTA.

### **Recommended Books**

1. G.D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley & Sons Ltd., Singapore (2003).
2. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2<sup>nd</sup> ed., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).

### **CH-332 Inorganic Chemistry-II (Cr. 2)**

**Chemistry of transition and inner transition elements:** Periodic trends, oxidation states, shapes of orbitals, metal-metal bonding, crystal field theory, magnetic properties, 3d, 4d and 5d transition series, 4f and 5f inner transition series, their coordination behavior etc. **Crystalline state:** ABAB- - - and ABCABC- - - packing, MX and MX<sub>2</sub> systems, **structure and energetics of inorganic molecules**, theory of metals and intermetallic compounds. **Redox reactions:** Balancing of redox reactions, mechanisms of electron transfer processes – outer sphere and inner sphere mechanism.

### **Recommended Books**

1. F.A. Cotton, et al., *Advanced Inorganic Chemistry*, 6<sup>th</sup> ed., John Wiley, New York (1999).
2. J.E. Huheey, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> ed., Addison-Wesley, Reading (1993).
3. M.C. Day Jr. and Jod Selbin, *Theoretical Inorganic Chemistry* by Reinhold Publishing Corporation, New York (1962).

### Supplementary Books

1. A.J. Emeleus and A.G. Sharp, *Modern Aspects of Inorganic Chemistry*, Read K. Paul, London (1983).
2. T. Moeller, *The Chemistry of the Lanthanides*, Chapman and Hall Ltd. London (1965).
3. J.D. Lee, *Concise Inorganic Chemistry*, Chapman and Hall London (1996).

### CH-332 Inorganic Chemistry Laboratory-II (Cr. 1)

Synthesis of selected coordination/organometallic compounds such as:

- |                        |                          |
|------------------------|--------------------------|
| i) $K_3[Cr(C_2O_4)_3]$ | ii) $[Co(NH_3)_5Cl]Cl_2$ |
| iii) $C_6H_4(OH)HgCl$  | vi) $(C_6H_4CH_2)_3SnCl$ |

Titrimetric and spectrophotometric determination of di and trivalent metal ions in complexes. Kinetics of inorganic chemical reactions such as reaction of iodine with persulphate.

### Recommended Books

1. A.I. Vogel, *A Textbook of Quantitative Inorganic Analysis: Theory and Practice*, Green and Co. Ltd., London (2000).
2. W.J. Jolly, *The Synthesis and Characterization of Inorganic Compounds*, Prentice Hall, Englewood Cliffs, New York (1970).

### 3<sup>rd</sup> and 4<sup>th</sup> Semester

#### CH-421 Principles and Applications of Molecular Spectrophotometry (Cr. 3)

**Molecular structure and spectral transitions:** Measurement of spectra, light scattering-elastic and inelastic, absorption and emission spectroscopy. **Absorption spectroscopy in UV-Visible region:** Absorbance and transmittance, applications and deviations of Beer-Lambert law, spectral resolution and errors in concentration measurements, applications and comparison of fluorescence and phosphorescence spectroscopy, spectral interferences and spectra of mixtures, chemical interferences, instrumental interferences. **Instrumentation:** Wavelength separations, sources and detectors for electromagnetic radiations. **Derivative spectroscopy:** Theory and applications. **IR and Raman spectroscopy:** Vibrational frequencies, qualitative analysis, IR spectra and Raman spectra, samples for IR and Raman spectroscopy, band intensities, quantitation, IR and Raman spectrophotometers, correlation charts and tables. **NMR Spectroscopy:** Introduction, principles and applications of NMR.

### Recommended Books

1. D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill Companies Inc. (2000).
2. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2<sup>nd</sup> ed., Wiley-VCH, Verlag GmbH & Co. KGaA, Weinheim (2004).

3. D.L. Pavia, G.M. Lampman, and G.S. Kriz, *Introduction to Spectroscopy*, 3<sup>rd</sup> ed., Thomson Learning Inc. (2001).

### Supplementary Books

1. K.A. Rubinson and J.F. Rubinson, *Contemporary Instrumental Analysis*, Prentice-Hall, Inc., USA (2000).
2. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Analysis*, 6<sup>th</sup> ed., Pearson Education Ltd. (2000).
3. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, *Fundamentals of Analytical Chemistry*, 8<sup>th</sup> ed., Thomson Books/Cole, Belmont, USA (2004).
4. F. Rouessac and A. Rouessac, *Chemical Analysis – Modern Instrumental Methods and Techniques*, John Wiley & Sons, Ltd., UK (2000).
5. G.D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley & Sons Ltd., Singapore (2003).
6. D.A. Skoog and J.J. Leary, *Principles of Instrumental Analysis*, 4<sup>th</sup> ed., Saunders College Publishing, USA (1992).
7. D.C. Harris, *Quantitative Chemical Analysis*, 5<sup>th</sup> ed., W.H. Freeman Company, New York (1999).

### **CH-422      Atomic Spectroscopy (Cr. 3)**

**Origin of spectral transitions in atoms:** Atomic spectra and spectral notations, intensities and line widths of gas-phase atomic spectra and its variations with temperature and pressure. **Absorption & emission spectra:** Boltzman distribution, spectral line broadening, background correction, factors affecting atomization/ionization. **Atomic absorption and emission methodologies:** Optimization of analytical conditions, concentration ranges in atomic spectroscopy. **Interferences:** Spectral, physical, chemical and instrumental and their elimination. **Optical components of atomic absorption/emission spectrophotometers:** Radiation sources, atomizers, monochromators and detectors, modulation in atomic spectroscopy. **Flame Vs. Electrothermal atomic absorption spectroscopy:** Qualitative and quantitative applications of absorption and emission measurements. **Flame photometry:** Flame characteristics and spectral interferences, components of flame photometer, non-metals and flame photometry. **Sampling:** Sample and standard preparation methods for atomic spectroscopy.

### Recommended Books

1. F. Rouessac and A. Rouessac, *Chemical Analysis – Modern Instrumental Methods and Techniques*, John Wiley & Sons, Ltd., UK (2000).
2. K.A. Rubinson and J.F. Rubinson, *Contemporary Instrumental Analysis*, Prentice-Hall, Inc., USA (2000).

3. R. Kellner, J.M. Mermet, M. Otto, M. Valcarcel and H.M. Widmer, *Analytical Chemistry*, 2<sup>nd</sup> ed., Wiley-VCH Verlag GmbH & Co. KGaA, Weinheim (2004).

### **Supplementary Books**

1. D.A. Skoog, D.M. West, F.J. Holler and S.R. Crouch, *Fundamentals of Analytical Chemistry*, 8<sup>th</sup> ed., Thomson Books/Cole, Belmont, USA (2004).
2. D. Harvey, *Modern Analytical Chemistry*, McGraw-Hill Companies Inc. (2000).
3. R.D. Braun, *Introduction to Instrumental Analysis*, McGraw-Hill Book Company (1987).
4. E.H. Evans, *An Introduction to Analytical Atomic Spectrometry*, John Wiley & Sons Ltd., New York (1998).
5. D.A. Skoog and J.J. Leary, *Principles of Instrumental Analysis*, 4<sup>th</sup> ed., Saunders College Publishing, USA (1992).
6. G.D. Christian, *Analytical Chemistry*, 6<sup>th</sup> ed., John Wiley & Sons Ltd., Singapore (2003).
7. J. Mendham, R.C. Denney, J.D. Barnes, and M. Thomas, *Vogel's Textbook of Quantitative Analysis*, 6<sup>th</sup> ed., Pearson Education Ltd. (2000).

### **CH-423      Advanced Analytical Chemistry (Cr. 2)**

**Thermal methods of analysis:** General introduction, principles, instrumentation, thermogravimetry, differential thermal analysis and differential scanning calorimetry, evolved gas detection, evolved gas analysis. **Applications:** Applications of thermal techniques in analysis of different materials.

### **Recommended Books**

1. T. Hatakeyama and F.X. Quinn, *Thermal Analysis: Fundamentals and Applications to Polymer Science*, Chichester, John Wiley & Sons (1999).
2. M.E. Brown, *Introduction to Thermal Analysis: Techniques and Applications*, Chapman and Hall, London (1988).
3. P.J. Haines, *Thermal Methods of Analysis: Principles, Applications and Problems*, Blackie Academic and Professional, London (1995).

### **Supplementary Books**

1. B. Wunderlich, *Thermal Analysis*, Academic Press, Boston (1990).
2. W.W.M. Wendlandt, *Thermal Methods of Analysis*, 3<sup>rd</sup> ed., John Wiley and Sons, New York (1986).
3. J.W. Dodd and K.H. Tonge, *Thermal Methods: Analytical Chemistry by Open Learning*, Chichester, John Wiley and Sons (1987).

### CH-427 Crystallography (Cr. 3)

**Introduction:** Techniques involving X-rays, historical background, the eye and microscope analogy, interatomic and intermolecular forces, solid-crystalline, amorphous. **X-rays:** Production, X-ray tubes, absorption and filtering, selection of radiation, detection of X-rays. **Geometry of the crystal:** Introduction, unit cells, lattices, crystal systems, crystal classes, space groups. **Symmetry:** Macroscopic and microscopic symmetry elements, crystal symmetry and properties. **Diffraction of X-rays:** Bragg's equation and Bragg's law, reciprocal lattice, Bragg's law in reciprocal lattice. **Diffractional methods:** Powder methods – camera and diffractometer, single crystal methods – camera (Rotation, Oscillation, Weissenberg and Precession) and diffractometer. Intensities of the diffracted beam; measurement, data reduction. Solution of the structure, refinement and interpretation of the result.

#### **Recommended Books**

1. B.D. Cullity and S.R. Stock, *Elements of X-ray Diffraction*, 3<sup>rd</sup> ed., Prentice Hall (2003).
2. L. Smart and M. Gagan, *The Molecular World: The Third Dimensions*, RSC, UK (2002).
3. M.M. Woolfon, *An Introduction to X-ray Crystallography*, Cambridge University Press (1970).

### CH-428 Organometallic Chemistry (Cr. 2)

Introduction: historical background and current trends. 18-Electron rule: rationalization, limitations. Types of ligands. Chemistry and bonding of metal-sigma and pi-complexes: metal carbonyls and related compounds, metal alkyls, metal hydrides, complexes of molecular nitrogen, oxygen and hydrogen, metal phosphines and complexes of pi-bond ligands. Applications of organometallic chemistry. Metal cluster and rationalization of their structures: electron counting schemes in clusters.

#### **Recommended Books**

1. R.H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, John Wiley & Sons (2014).
2. M. Bockmann, *Organometallic Chemistry 1 & 2*, Oxford Chemistry Primers (1994).
3. A. Yamamoto, *Organotransition Metal Chemistry: Fundamental Concepts and Applications*, John Wiley & Sons (1986).

### CH-429 Bio-coordination Chemistry (Cr. 2)

**Introduction: Elements and their role:** Essential and trace elements in biological systems, Roles of some individual elements in biological systems. **Cell and various elements:** Structure of cell and role of different metal ions in the cell. **Metals in**

**biological molecules:** Metal containing biological molecules and their function (hemes, Vit. B<sub>12</sub>, different enzymes, etc.)

### **Recommended Books**

1. R.W. Hay, *Bioinorganic Chemistry*, Ellis, Harwood, London (1991).
2. D.F. Fenton, *Bio-coordination Chemistry*, Oxford Primer Series (No.25), Oxford University Press (1995).
3. P.C. Wilkins and R.G. Wilkins, *Inorganic Chemistry in Biology*, Oxford Primer Series (No.46), Oxford University Press (1997).

### **Supplementary Book**

1. J. McMaster, *Annu. Rep. Prog. Chem., Sect. A*, 101, 607-630 (2005); 102, 564-583 (2006); 103, 492-517 (2007) (Reviews).

### **CH-430 Elementary Group Theory (Cr. 2)**

**Symmetry:** Symmetry, symmetry operations, point groups, **Groups and representations:** Groups, transformation, matrices, representations of groups, character tables. **Application:** Application of group theory to valence bond, molecular orbital, crystal field theories and IR spectra.

### **Recommended Books**

1. K.C. Molloy, *Group Theory for Chemists*, Harward Publishing Ltd. (2007)
2. F.A. Cotton, *Chemical Applications of Group Theory*, 3<sup>rd</sup> ed., John Wiley, New York (1990).
3. A.B.P. Lever, *Introduction to Electronic Spectroscopy*, Elsevier, Amsterdam (1968).
4. J.P. Facer, *Symmetry in Coordination Chemistry*, Academic Press, New York (1971).

### **Supplementary Books**

1. Alan and Vincent, *Molecular Symmetry and Group Theory*, John Wiley, London (1977).
2. J. Huheey, *Inorganic Chemistry: Principles of Structure and Reactivity*, 4<sup>th</sup> ed., Addison-Wesley, Reading/Singapore (1993).

### **CH-431 Coordination Chemistry (Cr. 3)**

**Introduction and historical development:** Introduction, Werner's coordination theory, nomenclature of the coordination complexes. **Bonding:** The electron pair bond, effective atomic number, electronic structure, bonding theories, magnetic properties. **Stereochemistry:** Geometry of coordination compounds, John-Teller distortions,

isomerism in metal complexes. **Preparation and reactions of coordination compounds:** Reactions in aqueous solution, in non-aqueous solvents, in the absence of solvent, thermal dissociation of solid complexes, oxidation-reduction reactions, catalysis, synthesis of cis-trans isomers, preparation of optically active compounds, carbonyls and organometallic compounds. **Complex ion stability:** Stability constant, factors that influence complex stability, determination of stability constants. **Kinetics and mechanisms of reactions of coordination compounds:** Rate of reaction, the rate law, effective collisions, inert and labile complexes, mechanisms of substitution reactions, octahedral substitution, square planar substitution, mechanisms of redox reactions.

Applications of coordination complexes in various fields.

### **Recommended Books**

1. F. Basolo and R.C. Johnson, *Coordination Chemistry*, NBF Pakistan (1988).
2. J.E. Huheey, *Inorganic Chemistry, Principles of Structure and Reactivity*, 4<sup>th</sup> ed., Addison-Wesley, Reading/Singapore (1993).
3. F.A. Cotton, et al., *Advanced Inorganic Chemistry*, 6<sup>th</sup> ed., John Wiley, New York (1999).

### **CH-432 Inorganic Chemistry-III (Cr. 2) (Compulsory)**

**Non-aqueous solvents:** Properties of ionizing solvents, classification, types of reactions, chemistry in non-aqueous solvents such as NH<sub>3</sub>, HF, CH<sub>3</sub>COOH, H<sub>2</sub>SO<sub>4</sub>, SO<sub>2</sub>, BrF<sub>3</sub>, N<sub>2</sub>O<sub>4</sub> etc. **Fused salts systems:** Reactions in molten salt systems (high temperature and low temperature molten salts). **Inorganic rings and cages:** Clathrates, inorganic rings, chains, cages of B, Si, N, P, S.

### **Recommended Books**

1. A.K. Holliday and A.G. Massey, *Inorganic Chemistry in non-aqueous solvents*, Pergamon Press Ltd. (1965).
2. H.H. Sisler, *Chemistry in Non-aqueous solvents*, Chapman & Hall Ltd. (1965).
3. J.E. Huheey, *Inorganic Chemistry, Principles of Structures and Reactivity*, 4<sup>th</sup> ed., Addison Wesley, Reading (1993).

### **CH-433 Inorganic Chemistry-IV (Cr. 2) (Compulsory)**

**Metal carbonyls:** Metal carbonyls, carbonyl hydrides, carbonyl chlorides, metal nitrosyls and related compounds. **Organometallic compounds:** Chemistry and bonding of metal-sigma and pi-complexes, fundamental processes in organometallic compounds, catalysis by organometallic compounds, complexes of molecular nitrogen and oxygen.

### **Recommended Books**

1. A. Yamamoto, *Organotransition Metal Chemistry: Fundamental Concepts and Applications*, John Wiley & Sons (1986).



2. P. Power, *Principles of Organometallic Chemistry*, 2<sup>nd</sup> ed., Chapman and Hall, London (1988).
3. R.H. Crabtree, *The Organometallic Chemistry of the Transition Metals*, 2<sup>nd</sup> ed., John Wiley & Sons (1994).

#### **CH-434 Inorganic Polymers (Cr. 2)**

**Inorganic Polymers:** Introduction to polymeric materials. Preparation of polyorganosiloxanes and various systems containing P-N; S-N and transition-metal polymers. **Characterization:** Characterization of polymeric materials (infrared, NMR, molecular weight determination, thermogravimetry, scanning electron microscopy). **Applications.**

#### **Recommended Books**

1. F.G.A. Stone and W.A.G. Graham, *Inorganic Polymers*, Academic Press, Inc., London (1962).
2. F.G.R. Gimblett, *Inorganic Polymer Chemistry*, Butterworths, London (1963).
3. C.E. Carraher, Jr., J.E. Sheads and C.U. Pittman, Jr., *Advances in Organometallic and Inorganic Polymer Science*, Marcel Dekker, Inc., New York (1982).

#### **Supplementary Book**

1. C.E. Carraher, Jr., *Polymer Chemistry*, 5<sup>th</sup> ed., Marcel Dekker, Inc., New York (2000).

#### **CH-436 Nuclear and Radiochemistry (Cr. 2)**

**Radioactivity:** Nuclear structure and properties. Radioactive decay. **Nuclear reactions.** Effect of radiation on biological systems. **Instrumentation:** Sources of nuclear bombarding particles. Detection and measurement of nuclear radiation. **Applications:** Application of radioactivity in various fields.

#### **Recommended Books**

1. K.H. Lieser, *Nuclear and Radiochemistry: Fundamentals and Applications*, 2<sup>nd</sup> rev. ed., Wiley-VCH, Berlin (2001).
2. G. Choppin, J.O. Liljenzin and J. Rydberg, *Radiochemistry and Nuclear Chemistry*, 3<sup>rd</sup> ed., Butterworth-Heinemann (2002).
3. Y. Hido and M. Satake, *An Introduction to Nuclear Chemistry*, Discovery Publishing House, New Delhi (2003).

#### **Supplementary Book**

1. G. Friedlander and J.W. Kennedy, *Nuclear Radiochemistry*, 3<sup>rd</sup> ed., John Wiley and Sons, New York (1981).

**Note:- In accordance with the policy of the department one of the following two courses (CH-435 and CH-437) will be offered in the third semester:**

**CH-435 Thesis/Research Project in Inorganic/Analytical Chemistry (Cr. 3)**

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

**CH-437 Inorganic/Analytical Chemistry Laboratory-III (Cr. 3)**

1. Analysis of Portland Cement.
2. Preparation and characterization of di- and tribenzyltin chloride.
3. Preparation and analysis of clathrate compound (benzene ammine nickel cyanide),  $\text{Ni}(\text{CN})_2 \cdot \text{NH}_3 \cdot \text{CH}_6$ .
4. Synthesis and characterization of inorganic compounds  $[\text{Co}(\text{NH}_3)_5\text{Cl}]$ ,  $[\text{Co}(\text{NH}_3)_5\text{NO}_2]$ .
5. Preparation and estimation of Grignard's reagent,  $\text{C}_2\text{H}_5\text{MgBr}$ .
6. Preparation of  $[\text{Cr}^{\text{II}}(\text{CH}_3\text{COO})_2] \cdot 2\text{H}_2\text{O}$ .
7. Synthesis and characterization of tetraphenyltin, triphenyltin chloride.
8. Synthesis and characterization of acetylacetonato metal complexes.
9. Synthesis and characterization of ferrocene.
10. Preparation of inorganic compounds and study of their optical activity,  $d, l[\text{trisethylenediamine Co(III)}]_3$ .

**Recommended Books**

1. W.J. Jolly, *The Synthesis and Characterization of Inorganic Compounds*, Prentice Hall, Englewood Cliffs, New York (1970).
2. J. Mendham, *Vogel's Textbook of Quantitative Chemical Analysis*, 6<sup>th</sup> ed., Pearson, India (2000).

**Note:- In accordance with the policy of the department one of the following two courses (CH-438 and CH-439) will be offered in the fourth semester:**

**CH-438 Research Project in Inorganic/Analytical Chemistry (Cr. 3)**

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

**CH-439 Advanced Inorganic/Analytical Chemistry Laboratory-IV (Cr. 3)**

The course teacher(s) shall offer advanced level practicals involving different experimental facilities available in the section/department. The details of the laboratory

work and the equipment involved shall be decided by the teacher concerned on the basis of the courses taught.

## II. Organic Chemistry

### 1<sup>st</sup> Semester

#### CH-341 Organic Chemistry-I (Cr. 3)

**Nomenclature of organic compounds:** Aliphatic and alicyclic hydrocarbons, oxygen and nitrogen containing compounds, monocyclic and bicyclic ring systems. **Literature of organic chemistry:** Primary sources, secondary sources, literature searching. **Introduction to stereochemistry:** Symmetry elements, chirality and stereoisomerism, nomenclature of chiral compounds, drawing Fischer projections, resolution of racemic mixtures. **Structure-reactivity relationship:** Changes in chemical reactivity with change in molecular structure in terms of acid base strength. **Reactive intermediates:** Types, structure, stability, methods of generation and their reactivity.

#### **Recommended Books**

1. J. McMurry, *Organic Chemistry*, 5<sup>th</sup> ed., Brooks/Cole, Boston (2007).
2. J.G. Smith, *Organic Chemistry*, McGraw-Hill, New York/Boston (2006).
3. L.G. Wade, *Organic Chemistry*, 5<sup>th</sup> ed., Pearson Education, Delhi (2003).

#### **Supplementary Books**

1. M.B. Smith and J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms, and Structure*, John Wiley & Sons (2007).
2. F.A. Carey, *Organic Chemistry*, McGraw-Hill, Higher Education, New York (2006).

#### CH-341 Organic Chemistry Laboratory-I (Cr. 1)

Experiments based on different techniques like re-crystallization, distillation, steam distillation, fractional distillation, vacuum distillation and different types of chromatography. Some one-step preparations of organic compounds.

#### **Recommended Books**

1. B.S. Furniss, *Vogel's Textbook of Practical Organic Chemistry Including Qualitative Organic*, Longman Group, London (1978)
2. R. Adams, J.R. Johnson and Wilcox Jr., *Laboratory Experiments in Organic Chemistry*, 6 Ed., Collier-M London (1970).

#### **Supplementary Books**

1. A.M. Schoffstall, and B.A. Gaddis, *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, (Druelinger, Melvin L.), McGraw-Hill, Boston (2004).

2. H. Becker and I. Hazzard, *Organicum: Practical Handbook of Organic Chemistry*, Reading, Masachuse Addison-Wesley Publishing Co. (1973).

## **2<sup>nd</sup> Semester**

### **CH-342 Organic Chemistry-II (Cr-3)**

**Functional Groups Chemistry:** Synthesis and reactions with mechanisms and stereochemical aspects. Hydrocarbons (Saturated, unsaturated, aromatic) alkyl halides, alcohols, phenols, ethers, amines, carbonyl compounds, carboxylic acids and their derivatives.

#### **Recommended Books**

1. F.A. Carey, *Organic Chemistry*, 6<sup>th</sup> ed., McGraw-Hill, Higher Education, Boston (2006).
2. J.G. Smith, *Organic Chemistry*, McGraw-Hill, Boston (2006).

#### **Supplementary Books**

1. T.W.G. Solomon and C.B. Fryhle, *Organic Chemistry*, 8<sup>th</sup> ed., John-Wiley, New York (2004).
2. L.G. Wade, *Organic Chemistry*, 5<sup>th</sup> ed., Pearson Education, New Delhi (2003).
3. M.A. Fox and J.K. Whitesell, *Organic Chemistry*, 3<sup>rd</sup> ed., Jones and Bartlett, Boston (2003).

### **CH-342 Organic Chemistry Laboratory-II (Cr. 1)**

One and two-step preparations of different types of organic compounds and their identification by physical and chemical methods.

#### **Recommended Books**

1. A.M. Schoffstall and B.A. Gaddis, *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, (Druelinger, Melvin L.), McGraw-Hill, Boston (2004).
2. R. Adams, JR. Johnson and Wilcox Jr., *Laboratory Experiments in Organic Chemistry*, 6<sup>th</sup> ed., Collier-M, London (1970).

#### **Supplementary Books**

1. B.S. Furniss, *Vogel's Textbook of Practical Organic Chemistry Including Qualitative Organic*, Longman Group, London (1978).
2. H. Becker and I. Hazzard, *Organicum: Practical Handbook of Organic Chemistry*, Reading, Masachuse Addison-Wesley Publishing Co. (1973).
3. J.C. Gilbert, and S.F. Martin, *Experimental Organic Chemistry: A Miniscale and Microscale Approach*, Saunders College Publishing, Fort Worth (1998).

## 3<sup>rd</sup> and 4<sup>th</sup> Semester

### CH-440 Chemistry of Heterocycles (Cr. 2)

**Heterocycles:** Introduction, significance and their uses. **Nomenclature:** Naming of heterocycles according to IUPAC, Hantzsch-Widmann- Pettersen system and SMILES. **Geometry and stereochemistry:** Saturated, unsaturated and aromatic heterocycles. aromaticity, tautomerism in small to large ring heterocycles. **Synthesis and reactions:** three-seven member heterocycles and fused ring heterocyclic systems.

#### **Recommended Books**

1. R.K. Bansel, *Heterocyclic Chemistry*, 4<sup>th</sup> ed., New Age International Pvt. Ltd., India (2005).
2. T. Eicher and S. Hauptmann, *The Chemistry of Heterocycles*, George Thieme Verlag, New York (1995).
3. J.A. Joule, K. Mills, G.F. Smith, *Heterocyclic Chemistry*, Stanley Thomes Publications. Ltd.; (1998).

#### **Supplementary Books**

1. R.H. Acheson, *An Introduction to Chemistry of Heterocycles*, John Wiley, New York (1987).
2. G.M. Loudon, *Organic Chemistry*, 4<sup>th</sup> ed., Oxford University Press, New York (2002).
3. M.A. Fox and J.K. Whitesell, *Organic Chemistry*, 3<sup>rd</sup> ed., Jones and Bartlett, Boston (2003).
4. M. Samisburg, *Heterocyclic Chemistry*, Royal Society Of Chemistry (2001)

### CH-441 Reaction Mechanism (Cr. 3)

**Introduction to reaction mechanism:** Basic concepts, energy profile diagrams, intermediate vs transition state and significance of reaction mechanism. **Methods of determination of reaction mechanism:** Identification of products, testing possible intermediates, trapping of intermediates, crossover experiments, isotopic labeling, stereochemical studies, catalysis and kinetic studies. **Mechanisms of different types of reactions:** Substitution, addition and elimination reactions.

#### **Recommended Books**

1. P. Sykes, *A Guidebook to Mechanism in Organic Chemistry*, 6<sup>th</sup> ed., Longman Scientific & Technical, London (1986).
2. M.B. Smith and J. March, *March's Advanced Organic Chemistry: Reactions, Mechanisms and Structure*, John Wiley & Sons, New York (2007).

3. B.K. Carpenter, *Determination of Organic Reaction Mechanisms*, John Wiley & Sons, New York (1984).

### Supplementary Books

1. T.H. Lowry and K.W. Richardson, *Mechanism and Theory in Organic Chemistry*, Harper & Row Publishers, New York (1987).
2. Jacobs, *Understanding Organic Reaction Mechanisms*, The University Press, Cambridge (1997).
3. M.G. Moloney, *Reaction Mechanisms at a Glance: a Stepwise Approach to Problem-Solving in Organic Chemistry*, Blackwell Science, Oxford (2000).
4. R. Bruckner, *Advanced Organic Chemistry: Reaction Mechanisms*, Harcourt Science, San Diego (2002).

### CH-442 Spectroscopic Methods in Organic Chemistry-I (Cr. 2)

**Introduction:** Fundamentals of spectroscopy. **UV-Visible spectroscopy:** Introduction, theory, instrumentation and sample handling. **Infra Red spectroscopy:** Introduction, theory, instrumentation and sample handling. **Mass spectrometry:** Introduction, theory, instrumentation and sample handling. **Applications:** Structure elucidation of simple organic molecules by UV, IR and MS.

### Recommended Books

1. R.M. Silverstein, F.X. Webster and D.J. Kiemle, *Spectrometric Identification of Organic Compounds*, John Wiley & Sons Inc., USA (2005).
2. D.L. Pavia, G.M. Lampman, and G.S. Kriz, *Introduction to Spectroscopy: a Guide for Students of Organic Chemistry*, Thomson Learning, Australia (2001).

### Supplementary Books

1. D.W. Brown, A.J. Floyed and M. Sainsbury, *Organic Spectroscopy*, I. Wiley and Sons, Chichester (1998).
2. D.H. Williams and I. Fleming, *Spectroscopic Methods in Organic Chemistry*, 4<sup>th</sup> ed., McGraw-Hill Book Co., London (1987).
3. M. Hesse, H. Nleir and U. Zech, *Spectroscopic Methods in Organic Chemistry*, Georg Thieme, Stuttgart, New York (1997).
4. Y.C. Ning, *Spectral Identification of Organic Compounds with Spectroscopic Techniques*, Wiley-VCH, Weinheim (2005).
5. M. Younas, *Organic Spectroscopy*, Ilmi Kitab Khana, Lahore (2004).

### **CH-443      Chemistry of Natural Products (Cr. 3)      (Compulsory)**

**Introduction:** Primary and secondary metabolites, isolation and structure elucidation by physical and chemical methods. **Partial and total synthesis:** Terpenoids, steroids, alkaloids, fatty acids and flavonoids.

#### **Recommended Books**

1. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University (2001).
2. J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthorpe and J.B. Harborne, *Natural Products*, Longman Group Ltd., U.K. (1994).
3. K. Nakanishi, T. Goto, S. Ioto, S. Natori, S. Nozone, et al., *Natural Products Chemistry*, Vol. 1, Academic Press Inc, New York (1974).

#### **Supplementary Books**

1. I.L. Finar, *Organic Chemistry: Stereochemistry and the Chemistry of Natural Products*, Vol. 2, Pearson Education, Delhi (1975).
2. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, 3<sup>rd</sup> ed., Chapman Hall, London (1993).

### **CH-444      Reaction Mechanism-II (Cr. 3)**

**Rearrangements:** Reactions involving 1,2 and non-1,2 rearrangements and their mechanism. **Oxidations:** Reactions involving removal of hydrogen, cleavage of C-C bond, replacement of hydrogen by oxygen, addition of oxygen and oxidative coupling along with their mechanisms. **Reductions:** Reactions involving replacement of oxygen by hydrogen, removal of oxygen, reductive cleavage and reductive coupling, selectivity in reductions. **Pericyclic reactions:** Introduction and significance, classification and their mechanistic analysis based on Woodward-Hoffmann rules and frontier orbitals method.

#### **Recommended Books**

1. J. March. *Advanced Organic Chemistry: Reaction, Mechanism and Structure*, 5<sup>th</sup> ed., John Wiley, New York (2007).
2. W. Caruthers, *Some modern Methods of Organic Synthesis*, 3<sup>rd</sup> ed., Cambridge University Press, Cambridge (1986).
3. F.L. Ansari, R. Quershi and M.L. Quershi, *Electrocyclic Reactions*, John Wiley & Sons (1999).

#### **Supplementary Books**

1. R.O.C. Norman, *Principles of Organic Synthesis*, 3<sup>rd</sup> ed., Chapman and Hall, London (1993).

2. R.T. Morrison and R.N. Boyd, *Organic Chemistry*, 6<sup>th</sup> ed., Prentice Hall, New Jersey (1992).
3. P. Sykes, *A Guide Book to Mechanism in Organic Chemistry*, 6<sup>th</sup> ed., Longman Scientific and Technical, London (1986).

#### **CH-445 Stereochemistry (Cr. 3) (Compulsory)**

**Introduction:** History and significance. **Static stereochemistry:** Structure and symmetry, conformations and configurations, methods for determination of relative and absolute configuration, stereochemical nomenclature. **Types of chirality:** Central, axial and planar chiral compounds, atropisomerism, molecular overcrowding and cyclostereoisomerism. **Dynamic stereochemistry:** Stereochemical reactions, stereoselectivity and stereospecificity, prostereoisomerism and prochirality. **Analytical methods:** Determination of enantiomer and diastereomer composition using chiroptical, chromatographic and NMR spectroscopic methods. **Resolution:** Diastereoisomer formation, chiral derivatization agents (CDAs), chiral resolving agents (CRAs), chromatographic, kinetic, mechanical and enzymatic resolutions, preferential crystallization.

#### **Recommended Books**

1. E.L. Eliel, S.H. Wilen, M.P. Doyle, and P. Michael, *Basic Organic Stereochemistry*, Wiley Interscience, New York (2003).
2. P.S. Kalsi, *Stereochemistry and Mechanism through Solved Problems*, New Age International Publishers, New Delhi, India (2001).
3. K. Mislow, *Introduction to Stereochemistry*, W.A. Benjamin, New York (1966).

#### **Supplementary Books**

1. J. Eames (Queen Mary and Westfield College, University of London) and J.M. Peach, *Stereochemistry at a Glance*, Blackwell Publishing (2003).
2. D.G. Morris, *Stereochemistry*, Royal Society of Chemistry, U.K (2001).
3. M. North, *Principles and Applications of Stereochemistry*, Stanley Thornes: Cheltenham, UK (1998).

#### **CH-446 Retrosynthesis (Cr.3)**

**Introduction to retrosynthesis:** Concepts of synthons and retrosynthetic approach. **Synthesis and uses:** alkyl halides, alkenes, alkynes, alcohols, ethers, aromatic compounds, carbonyl and nitrogen compounds. **Bond formations:** C-C, C-N, and C-O bond formation. **Difunctionalised compounds:** 1,2; 1,3; 1,4; 1,5; and 1,6. **Cyclizations:** Simple intramolecular reactions such as aldol, claisen condensation and robinson annulation reaction leading to cyclic structures. **Application:** Application of the concepts to various target molecules.



### **Recommended Books**

1. S. Warren, *Organic Synthesis: The Disconnection Approach*, John Wiley and Sons, Chichester (1992).
2. R.O.C. Norman and J.M. Coxon, *Principles of Organic Synthesis*, Blackie Academic and Professional, London (1993).
3. J. Clayden, N. Greeves, S. Warren and P. Wothers, *Organic Chemistry*, Oxford University (2001).

### **Supplementary Books**

1. C. Willis and M. Willis, *Organic Synthesis*, Oxford Science Press (1995).
2. G.D. Meakins, *Functional Groups: Characteristics and Interconversions*, Oxford Science Press (1996).

**Note:- In accordance with the policy of the department one of the following two courses (CH-447 and CH-448) will be offered in the third semester:**

#### **CH-447      Organic Chemistry Laboratory-III (Cr. 3)**

Multistep synthesis of different types of organic compounds, purification and identification of synthesized compounds by physical and chemical methods.

### **Recommended Books**

1. B.S. Furniss, *Vogel's Textbook of Practical Organic Chemistry Including Qualitative Organic*, Longman Group, London (1978).
2. H. Becker and I. Hazzard, *Organicum: Practical Handbook of Organic Chemistry*, Reading, Masachuse Addison-Wesley Publishing Co. (1973).
3. R. Adams, J.R. Johnson and Wilcox Jr., *Laboratory Experiments in Organic Chemistry*, 6<sup>th</sup> ed., Collier-M, London (1970).

### **Supplementary Books**

1. A.M. Schoffstall, and B.A. Gaddis, *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, (Druelinger, Melvin L.), McGraw-Hill, Boston (2004).
2. J.C. Gilbert, and S.F. Martin, *Experimental Organic Chemistry: a Miniscale and Microscale Approach*, Saunders College Publishing, Fort Worth (1998).

#### **CH-448      Thesis/Research Project in Organic Chemistry (Cr. 3)**

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

**Note:- In accordance with the policy of the department one of the following two courses (CH-449 and CH-475) will be offered in the fourth semester:**

**CH-449      Advanced Organic Chemistry Laboratory-IV (Cr. 3)**

Synthesis and characterization of some commercially important polymers, isolation, purification and identification of natural products, synthesis of some pharmaceutically important heterocyclic compounds.

**Recommended Books**

1. A.M. Schoffstall, and B.A. Gaddis, *Microscale and Miniscale Organic Chemistry Laboratory Experiments*, (Druelinger, Melvin L.), McGraw-Hill, Boston (2004).
2. B.S. Furniss, *Vogel's Textbook of Practical Organic Chemistry Including Qualitative Organic*, Longman Group, London (1978).
3. R. Adams, J.R. Johnson and Wilcox Jr., *Laboratory Experiments in Organic Chemistry*, 6<sup>th</sup> ed., Collier-M, London (1970).

**Supplementary Books**

1. H. Becker and I. Hazzard, *Organicum: Practical Handbook of Organic Chemistry*, Reading, Masachuse Addison-Wesley Publishing Co. (1973).
2. J.C. Gilbert, and S.F. Martin, *Experimental Organic Chemistry : a Miniscale and Microscale Approach*, Saunders College Publishing, Fort Worth (1998).

**CH-475      Thesis/Research Project in Organic Chemistry (Cr. 3)**

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

**CH-470      Biochemistry (Cr. 2)**

**Chemistry and metabolism of biopolymers:** carbohydrates, proteins, nucleic acids. **Chemistry of lipids:** fatty acids, eicosanoids, triglycerols, glycerophospholipids, sphingolipids, glycolipids, steroids and waxes. **Enzymes:** Classification, nomenclature, kinetics, mechanism of action and enzyme inhibition.

**Recommended Books**

1. D. Voet and J. Voet, *Biochemistry*, 2<sup>nd</sup> ed., John Wiley, New York (1995).
2. I.L. Finar, *Organic Chemistry, (Stereochemistry and the Chemistry of Natural Products)*, Vol. II, Pearson Education, New Delhi (1975).

**Supplementary Books**

1. T. Delvin, *Textbook of Biochemistry*, 4<sup>th</sup> ed., John Wiley, New York (1997).
2. J. Mann, R.S. Davidson, J.B. Hobbs, D.V. Banthrope and J.B. Harborne, *Natural Products*, Longman Group Ltd., U.K. (1994).

3. M. Hem, L.R. Best and S. Pattison, *Introduction to General, Organic, and Biochemistry*, Susan Arena, Wiley (2004).
4. D. Voet, J.G. Voet, *Fundamentals of Biochemistry: Life at the Molecular Level*, Charlotte W. Pratt, Wiley (2005).
5. F.A. Bettelheim, W.H. Brown and M.K. Campbell, *Introduction to General, Organic and Biochemistry*, Shawn O. Farrell, Brooks Cole (2006).

#### **CH-471 Name Reactions (Cr-2)**

**Recent developments, mechanistic, stereochemical aspects and synthetic applications of various Name reactions:** Aldol Condensation, Micheal Addition, Knoevenagal Condensation, Claisen Condensation, Dickmann Condensation, Mannich Reaction, Wittig Reaction, Peterson Reaction, Heck Reaction, Friedel-Craft Alkylation, Acylation and Related Reactions, Favorski Rearrangement, Hunsdiecker Reaction And Fischer Indole Synthesis.

#### **Recommended Book**

1. B.P. Mundy, M.G. Ellerd, F.G. Favalozo and F.G Favalozo, jr., *Name Reactions and Reagents in Organic Synthesis*, John Wiley, New York (2005).

#### **Supplementary Books**

1. M.B. Smith, *March's Advanced Organic Chemistry: Reactions, Mechanism and Structure*, 5<sup>th</sup> ed., John Wiley, New York (2001).
2. R.O.C. Norman, *Principles of Organic Synthesis*, 3<sup>rd</sup> ed., Chapman-Hall, London (1993).

#### **CH-472 Introduction to Polymer Chemistry (Cr.3)**

**Introduction:** Definition, nomenclature. **Classification of polymers:** Thermoplastics, thermosets, elastomers, rubbers etc. **Types of polymerization reactions:** Step growth, chain growth, free radical, ionic polymerizations, co-polymerization. **Characterization of polymers:** Spectroscopic methods such as infra red, nuclear magnetic resonance; Thermal methods such as differential scanning calorimetry, thermal gravimetric analysis, thermo mechanical and some physico-chemical methods.

#### **Recommended Books**

1. F.W. Billmeyer, *Textbook of Polymer Science*, Interscience (1994).
2. G. Odian, *Principles of Polymerization*, 3<sup>rd</sup> ed., John Wiley & Sons (2004).

#### **Supplementary Books**

1. H.R. Ailcock and F.W. Lampe, *Contemporary Polymer Chemistry*, 4<sup>th</sup> ed., Prentice Hall (2003).

2. M.S. Bhatnagar, *A Textbook of Polymers*, Vol. I, II, III, S. Chand & Co. Ltd. (2004).
3. J.R. Fried, *Polymer Science & Technology*, Prentice Hall, Inc. (1995).

### **CH-473 Quantum Organic Chemistry (Cr. 2)**

**Basic concepts:** Wave-particle duality, properties of wave function and wave equation. **Hückel molecular orbital method (HMO):** Hückel systems, HMO relationship and energy level patterns of linear and cyclic conjugated polyenes. **Applications of HMO results:** Correlation of HMO results with molecular properties, prediction and interpretation of IR, UV spectra, chemical reactivity and reaction mechanism by using HMO software.

#### **Recommended Books**

1. F.L. Ansari, R. Quershi and M.L. Quershi, *Electrocyclic Reactions*, John Wiley & Sons (1999).
2. C.M. Quinn, *Computational Quantum Chemistry*, Academic Press (2002).
3. K. George, *Introductory Organic Quantum Chemistry*, Academic Press, New York (1962).
4. R.A Jackson, *Mechanism in organic reactions*, Royal Society of Chemistry (2004).

#### **Supplementary Books**

1. D. Young, *Computational Chemistry: A practical Guide for Applying Techniques to Real World Problems*, Wiley Interscience (2001).
2. F. Jonsen, *Introduction to Computational Chemistry*, John Wiley (1999).
3. E. Lewars, *Computational Chemistry*, Kluwer Academic Press (2003).
4. C.J. Cremer, *Essentials of computational Chemistry*, JW. (2004).

### **CH-474 Spectroscopic Methods in Organic Chemistry-II (Cr. 3) (Compulsory)**

**Nuclear magnetic resonance:** Introduction, theory, instrumentation and sample handling. **Chemical shifts:** Chemical shifts in  $^1\text{H}$ - and  $^{13}\text{C}$ -NMR, factors affecting chemical shifts, chemical shift equivalence and magnetic equivalence. **Spin couplings:** Spin couplings and factors affecting spin couplings, first order spin systems. **Double resonance experiments:** Selective spin decoupling, nuclear overhauser effect. NOE difference spectra,  $^1\text{H}$  BB decoupled and DEPT spectra. **Applications:** Shift reagents, dynamic NMR, stereochemical assignments in different types of compounds, NMR in biochemistry and medicine, structure elucidation of organic compounds by joint applications of UV, IR, NMR and MS.

### Recommended Books

1. M. Hesse, H. Meier and B. Zeeh, *Spectroscopic Methods in Organic Chemistry*, Georg Thieme Verlag, Stuttgart, Germany (1997).
2. D.L. Pavia, G.M. Lampman and G.S. Kirz, *Introduction to Spectroscopy*, Brooks/Cole Thomson Learning, USA (2001).
3. R.M. Silverstein, F.X. Webster and D.J. Kiemle, *Spectrometric Identification of Organic Compounds*, John Wiley & sons Inc., USA (2005).

### Supplementary Books

1. L.M. Harwood and T.D.W. Claridge, *Introduction to Organic Spectroscopy*, Oxford University Press Inc., New York (1997).
2. R.S. Macomber, *NMR Spectroscopy: Basic Principles and Applications*, Harcourt Brace Jovanovich Publishers, San Diego (1988).
3. H. Friebolin, *Basic one-and two-dimensional NMR spectroscopy*, 4<sup>th</sup> ed., Wiley-VCH, New York (2005).
4. J.K.M. Sanders and B.K. Hunter, *Modern NMR Spectroscopy: a Guide for Chemists*, The University Press, Oxford (1993).
5. E. Breitmaier, *Structure Elucidation by NMR in Organic Chemistry: a Practical Guide*, John Wiley, West Sussex (2002).
6. M. Younas, *Organic Spectroscopy*, Ilmi Kitab Khana, Lahore (2004).
7. Y.C. Ning, *Spectral Identification of Organic Compounds with Spectroscopic Techniques*, Wiley-VCH, Weinheim (2005).
8. C.J. Creswell, O.A. Runquist and M.M. Campbell, *Spectral Analysis of Organic Compounds*, 2<sup>nd</sup> Edition, Longman, London (1972).

## III. Physical Chemistry

### 1<sup>st</sup> Semester

#### CH-050 Basic Mathematics for Chemistry (Cr. 2)

**Review of basic algebra:** Constants and variables; complex numbers. **Equations:** Linear, quadratic and higher order; roots of equations. **Functions:** Linear, polynomial, exponential, logarithmic, trigonometric. **Coordinate systems:** Cartesian, polar, their relationship; graphs, axes, scale, straight line, curves. **Differentiation:** Single variable problems, concept of maxima and minima, partial differentiation. **Integration:** indefinite and definite, determination of unknown constant; problems of multiple variables. **Matrices and determinants:** Vectors. The above contents with specific applications to chemical problems.

### Recommended Books

1. G. Doggett and B.T. Sutcliff, *Mathematics for Chemistry*, Longman Scientific & Technical, New York (1995).
2. P. Abbott, *New Calculus*, Teach Yourself Books, Hodder and Stoughton (1984).

3. F. Daniels, *Mathematical Preparation for Elementary Physical Chemistry*, McGraw-Hill, New York (1986).
4. K.J. Smith, *Algebra and Trigonometry*, Brooks/Cole Publishing Company, California (1987).
5. K.J. Smith, *Calculus with Applications*, Brooks/Cole Publishing Company, California (1988).
6. J. Barrante, *Applied Mathematics for Physical Chemistry*, Prentice Hall, Inc. (1974).

### **CH-351 Physical Chemistry-I (Cr. 3)**

**Gases:** Ideal and real gases; Virial coefficients; van der Waals equation; transport properties; distribution of energies and speeds; molecular collisions and collision theory. **Thermodynamics:** Laws of thermodynamics. Concepts of enthalpy, entropy, heat capacity, free energy and process reversibility. Applications of thermodynamics to chemical systems. **Chemical kinetics:** Reactions and reaction rate laws, order of reaction, experimental determination of reaction orders, factors influencing reaction rates, elementary reactions and reaction mechanism. Reactions with simple kinetic form; 0<sup>th</sup>-order, 1<sup>st</sup>-order, 2<sup>nd</sup>-order, complex reactions. **Electrochemistry and solutions:** Ideal and non-ideal solutions; electrolyte solutions and types of interactions. Ionic activity; ionic equilibria; electrode potentials. Redox reactions; electrochemical cells. Nernst equation.

#### **Recommended Books**

1. P.W. Atkins, *Physical Chemistry*, 7<sup>th</sup> ed., Freeman & Co., New York (2005).
2. R.A. Alberty and R.J. Silby, *Physical Chemistry*, John Wiley, New York (1995).
3. I.N. Levine, *Physical Chemistry*, McGraw Hill, New York (2002).

#### **Supplementary Books**

1. J.H. Espenson, *Chemical Kinetics and Reaction Mechanisms*, 2<sup>nd</sup> ed., McGraw-Hill, Singapore (1995).
2. J.L. Latham and A.E. Burgess, *Elementary Reaction Kinetics*, 3<sup>rd</sup> ed., John Wiley, New York (1981).
3. P.W. Atkins, *Elements of Physical Chemistry*, W.H. Freeman and Company, New York (1996).

### **CH-351 Physical Chemistry Lab-I (Cr. 1)**

1. Handling of chemicals and preparation of standard solutions.
2. To determine the rate constant for the acid catalyzed reaction of hydrolysis of an ester.

- Determination of molar refraction of different pure liquids and binary mixtures. ( $\text{H}_2\text{O}$ ,  $\text{CH}_3\text{OH}$ ,  $\text{C}_2\text{H}_5\text{OH}$ ,  $\text{C}_3\text{H}_7\text{OH}$ )
- Determination of equivalence point in acid-base titration using pH meter.
- Determination of molar mass of a given compound using cryoscopic method.
- Adsorption study of an organic acid on charcoal using adsorption isotherm.
- Determination of distribution constant for heterogeneous equilibrium using Nernst's distribution law.
- Determination of activation energy of a chemical reaction.
- Calorimetric determination of the heat of neutralization of a strong acid and a strong base.
- Spectroscopic characterization and study of Beer's law.

#### **Recommended Books**

- C.W. Garland, J.W. Nibler and D.P. Shoemaker, *Experiments in Physical Chemistry*, McGraw Hill, 7<sup>th</sup> ed. (1996).
- A Findlay, *Findlay's Practical Physical Chemistry*, Longman, London (1972).

#### **Supplementary Book**

- D.A. Skoog, *Principles of Instrumental Analysis*, 3<sup>rd</sup> ed., Harcourt Brace College Pub., New York (1998).

### **2<sup>nd</sup> Semester**

#### **CH-352 Physical Chemistry-II (Cr. 3)**

**Quantum mechanics:** Historical background of the development in atomic structure; basic concepts of quantum mechanisms; wave functions; vectors; operators; eigen values. Schrödinger's equation and its application to simple system: particle in one- and three dimensional box; rigid rotor; hydrogen atom and hydrogen-like ions; quantum numbers. **Chemical bonding:** Molecular systems:  $\text{H}_2$ -molecule. Molecular orbital (MO) and Valence bond (VB) theories; hybridization. **Molecular spectroscopy:** Rotational, vibrational and electronic spectroscopy of diatomic molecules; basic nuclear magnetic resonance spectroscopy.

#### **Recommended Books**

- I.N. Levine, *Physical Chemistry*, 5<sup>th</sup> ed., Tata McGraw-Hill (2002).
- P.W. Atkins and J. de Paula, *Physical Chemistry*, 7<sup>th</sup> ed., Oxford University Press (2002).

#### **Supplementary Books**

1. H. Kuhn and H.D. Fosterlings, *Principles of Physical Chemistry*, John Wiley & Sons, Ltd. (2000).
2. D.O. Hayward, *Quantum Mechanics for Chemists*, Royal Society for Chemistry (2002).

### **CH-352 Physical Chemistry Lab-II (Cr. 1)**

1. Conductometric determination of degree of dissociation and dissociation constant of a weak acid.
2. Determination of the equilibrium constant for the reversible reaction,  $I_2 + I^- \leftrightarrow I_3^-$ .
3. Determination of heat of solution of oxalic acid by solubility method using van't Hoff equation.
4. Determination of the specific rate constant for the saponification of ethylacetate conductometrically.
5. Spectrophotometric determination of dissociation constant and  $pK_a$  value of an indicator.
6. Determination of specific angle of rotation of sucrose using a polarimeter.
7. To determine the degree of hydrolysis, hydrolysis constant and dissociation constant for acetic acid from the hydrolysis of sodium acetate in aqueous solution.
8. Determination of molar volumes of the given liquids and investigation of solvent-solvent interaction from the density measurements of their mixtures.
9. Determination of equivalence point in acid-base titration using conductivity meter.
10. Comparison of molar conductivity for 1:1 electrolytes and verification of Debye-Huckel-Onsager equation.

### **Recommended Books**

1. C.W. Garland, J.W. Nibler and D.P. Shoemaker, *Experiments in Physical Chemistry*, McGraw Hill, 7<sup>th</sup> ed. (1996).
2. A. Findlay, *Findlay's Practical Physical Chemistry*, Longman, London (1972).

### **Supplementary Books**

1. D.A. Skoog, *Principles of Instrumental Analysis*, 3<sup>rd</sup> ed., New York (1998).
2. L.P. Gold, L. Gold, *Physical Chemistry Laboratory*, Primis Publishers (1997). ISBN: 0072902698.



### 3<sup>rd</sup> and 4<sup>th</sup> Semester

*Note:- All the 3 credit Physical Chemistry courses of M.Sc. 3<sup>rd</sup> and 4<sup>th</sup> semesters are compulsory.*

#### CH-450 Computational Chemistry (Cr. 2)

**Computer aided numerical methods:** Least square curve fitting method for linear functions and its modified forms for other functions, statistical analysis. Numerical differentiation. **Geometrical application of integration:** Area under the curves of various natures, calculation of volume, length of curve line. Numerical integration: Rectangular, trapezoidal and parabolic methods of approximation. **Molecular modeling:** Model building using different force field parameters, geometry optimization.

#### **Recommended Books**

1. K. Smith, *Calculus with Applications*, Brooks/Cole, Pacific Grove (1998).
2. R. Kumari, *Computers and Their Applications to Chemistry*, Narose Publishing House, New Delhi, India (2005).
3. R.J. Mortimer, *Mathematics for Physical Chemistry*, 3<sup>rd</sup> ed., Elsevier Academic Press (2005).

#### **Supplementary Books**

1. E. Lewars, *Computational Chemistry, Introduction to the Theory and Application of Molecular and Quantum Mechanics*, Kluwer Academic Publishers, Boston (2003).
2. J. Pachner, *Handbook of Numerical Analysis Applications*, McGraw-Hill, New York (1984).

#### CH-451 Chemical Kinetics (Cr. 3)

**Transition state theory:** Temperature effects; heat capacity of activation; composite rate constants; pressure effects and volume of activation; interpretation of activation parameters. **Reaction mechanisms:** Mechanistic interpretation of rate laws, equivalent kinetic expressions, kinetically indistinguishable schemes, pH- rate profiles. **Composite reactions:** Reversible 1<sup>st</sup> and higher order reactions, parallel and concurrent reactions, consecutive first order reactions; steady state approximation; rate controlling step; catalyzed and enzyme catalyzed reactions. **Chain reactions:** Decomposition of acetaldehyde; autoxidation of an organo-chromium complex. **Fast reactions:** Flow methods for rapid reactions, shock wave methods, chemical relaxation methods, quenching by fluorescence method, flash and laser photolysis.

#### **Recommended Books**

1. J.H. Espenson, *Chemical Kinetics and Reaction Mechanisms*, 2<sup>nd</sup> ed., McGraw Hill, Singapore (1995).
2. A.A.M. Frost and R.G. Pearson, *Kinetics and Mechanism*, 3<sup>rd</sup> ed., Butterworths,

London (1969).

### Supplementary Books

1. I.N. Levine, *Physical Chemistry*, McGraw Hill, New York (2002).
2. K.J. Laidler, *Chemical Kinetics*, 3<sup>rd</sup> ed., Pearson Education Ins., Singapore (1987).
3. S.R. Logan, *Fundamentals of Chemical Kinetics*, Longman Group Limited (1996).

### CH-452 Quantum Chemistry (Cr. 3)

**Basic postulates and theorems of quantum mechanics. Operators:** Hermetian angular momentum; eigen function, eigen values and eigen value equation. **Quantum mechanical treatment (solution of Schrödinger equation) of some representative systems:** Particle in three-dimensional box; harmonic oscillator; rigid rotor; hydrogen like atoms. **Treatment of many electron atoms:** Paulis' principle; Hund's rule; spin-orbit interaction. Variation method. Perturbation theory. Molecular symmetry. **Chemical bonding:** Valence bond (VB) and molecular orbital (MO) theories, HMO calculation and band gap theory.

### Recommended Books

1. D.O. Hayward, *Quantum Mechanics for Chemists*, Royal Society of Chemistry, UK (2002).
2. J.P. Lowe, *Quantum Chemistry*, 2<sup>nd</sup> ed., Academic Press, New York (1993).
3. D.A. McQuarie, *Quantum Chemistry*, Oxford University Press, Oxford, UK (1983).

### Supplementary Books

1. F.L. Pilar, *Elementary Quantum Mechanics*, 2<sup>nd</sup> ed., McGraw Hill, New York (2001).
2. I.N. Levine, *Quantum Chemistry*, 4<sup>th</sup> ed. Prentice Hall, New Delhi (1991).

### CH-453 Molecular Spectroscopy (Cr. 3)

**Introduction:** Principles and classification of spectroscopy; interaction of light and matter; de-excitation modes; various spectra and their characterization. **Rotational spectroscopy:** classification of molecules; diatomic rigid and non-rigid molecules; polyatomic linear molecules; symmetric tops; applications. **Vibrational spectroscopy:** Classification of vibrational modes; diatomic molecules; diatomic vibrating-rotator; breakdown of the Born-Oppenheimer approximation; polyatomic linear vibrators and vibrating symmetric tops. **Electronic spectroscopy of diatomic molecules:** Vibrational coarse structure; the Frank-Condon principle and dissociation. **Nuclear magnetic resonance spectroscopy:** Principles; applications.

### Recommended Books

1. C.N. Banwell, *Fundamentals of Molecular Spectroscopy*, 3<sup>rd</sup> ed., McGraw-Hill, UK (1983).
2. G.M. Barrow, *Introduction to Molecular Spectroscopy*, McGraw-Hill (International Student Edition) (1990).
3. G. Aruldas, *Molecular Structure and Spectroscopy*, Prentice-Hall (India) (2004).
4. H. Friebolin, *Basic One- and Two- Dimensional NMR Spectroscopy*, VCH, Weinheim (1993).

### CH-454 Chemical Thermodynamics (Cr. 3)

**Basic concepts:** Relations used in thermodynamics, free energy, enthalpy, entropy, laws of thermodynamics. **Systems of variable compositions:** Mixtures of gases; the fugacity function; partial molal quantities; ideal solutions. **Laws of dilute solutions:** Henry's law; Nernst's distribution law; Raoult's law; activity and activity coefficients; equilibrium constants; free energy changes in solutions. **Colligative properties:** Vapour-pressure lowering, freezing point depression, elevation of boiling point and osmotic pressure. **Phase rule:** Phase equilibrium, one component system, multicomponent systems.

### Recommended Books

1. I.M. Klotz, *Chemical Thermodynamics*, 3<sup>rd</sup> ed., W.A. Benjamin Inc., California; (1972).
2. I.N. Levine, *Physical Chemistry*, McGraw Hill, New York (2002).

### Supplementary Books

1. K.S. Pitzer, *Thermodynamics*, 3<sup>rd</sup> ed. McGraw-Hill, New York (1995).
2. J.B. Ott and J.B. Goates, *Chemical Thermodynamics*, Elsevier, New York (2000) ISBN: 0125309902.
3. D.A. McQuarrie and J D Simon, *Molecular Thermodynamics*, Viva Books, Pvt. Ltd., New Delhi (2004).

### CH-455 Statistical Mechanics (Cr. 2)

**Historic background and basics:** Probability; description of various systems; ensembles; concepts of states and accessible states; distribution of energy; Maxwell-Boltzmann's statistic (MBS) of the systems of independent particles. **Partition functions:** Derivations and determinations for simple molecules. **Statistical thermodynamics:** Correlation of partition functions and thermodynamic functions. **Applications:** To chemical equilibrium and chemical kinetics; Fermi-Dirac's (FD) and Bose-Einstein's (BE) statistics.

### Recommended Books

1. R. Reif, *Statistical Physics*, McGraw-Hill Book Co., New York (1967).
2. D.A. McQuarrie and J.D. Simen, *Physical Chemistry (A molecular approach)*, Viva Books Pvt. Ltd., New Delhi (2004).
3. Fritz & Fritz, *Statistical Thermodynamics*, Wiley, New York (1959).
4. J.M. Seddon and J.D. Gale, *Thermodynamics and Statistical Mechanics*, RSC Publishers (2001).
5. K. Nash, *Elements of Classical and Statistical Thermodynamics*, Addison-Wesley Publishing Company, London (1970).
6. Sears and W. Francis, *Thermodynamics, Kinetic Theory and Statistical Thermodynamics*, Addison and Wile, London (1975).

### CH-456 Nuclear and Radiation Chemistry (Cr.2)

**Fundamentals:** Brief history, transformation hypothesis, electron- proton hypothesis. **Properties of nucleus:** Sub-atomic particles; leptons, baryons, mesons, quarks. Nuclear size and density; types of nuclides: isobars, isotones, isomers; mass defect and binding energy. Half-life. **Models of nuclear structure:** Nuclear force radii, liquid drop model, shell model. **Equations of decay and growth processes:** successive decay, branched decay; transient and secular equilibria. **Radioactivity:** Types of nuclear reactions:  $\alpha$ -decay,  $\beta$ -decay, positron emission, electron capture and their thresholds. Applications of nuclear chemistry.

### Recommended Books

1. G. Friedlander and W Kennedy, *Nuclear and Radiochemistry*, John Wiley & Sons, New York (1981).
2. K.H. Lieser, *Nuclear and Radiochemistry (Fundamentals and Applications)*, John Wiley-VCH Weinheim (2001).

### Supplementary Books

1. H.J. Arnikar, *Essentials of Nuclear Chemistry*, New Age International publishers Ltd. Wiley Eastern Ltd., New Delhi (1995).
2. G.R. Choppin, J.O. Liljenzin and J. Rydberg, *Radiochemistry and Nuclear Chemistry*, Butter worth-Heinemann, USA (2002).

### CH-457 Solid State Chemistry (Cr. 2)

**Unit cells and crystal systems:** Lattices and their description: Bravais lattice; Miller indices; unit cell contents. Point groups and their relevant classification based on symmetry. **Space groups and crystal structures:** Close-packed structures (cubic, hexagonal, tetragonal and other packing arrangements). Important structure types (Rutile, Rock Salt, Zinc Blend, Wurtzite. etc). **Perfect and imperfect crystals:** Types of defects

with description. Diffusion of ions in solids; dislocation; mechanical properties and reactivity of solids. **Theories of electrical conductance:** Different types of solids, metals and non-metals.

#### **Recommended Books**

1. A.R. West, *Solid State Chemistry*, 2<sup>nd</sup> ed. John Wiley, Singapore (2002).
2. W.J. Moore, *Seven Solid States*, W.A. Benjamin Inc., New York (1967).
3. R.H. Bube, *Electrons in Solids*, 3<sup>rd</sup> ed., Academic Press, San Diego (1992).

#### **Supplementary Books**

1. W.D. Callister, *Material Science and Engineering*, 6<sup>th</sup> ed. John Wiley, New York (2003).
2. *Electronic Materials Handbook*, Vol. I, Packaging, ASM International Materials Park, Ohio (1989).
3. R.E. Hummel, *Electronic Properties of Materials*, 3<sup>rd</sup> ed. Springer-Verlag, New York (2000).

#### **CH-458 Solution Chemistry (Cr. 2)**

**Solutions:** Their role in chemistry; classification; concept of solute and solvent; mixtures and their importance. **Interactions in solutions:** Solvent-solvent interactions; solute-solvent interactions. **Electrolyte solutions:** Ion-ion interactions; ion-pairing; structure of solvates. **Measurement:** Microscopic and macroscopic properties: transport properties.

#### **Recommended Books**

1. J. Burgess, *Metal Ions in Solutions*, 2<sup>nd</sup> ed., Ellis Harwood Ltd. UK (1978).
2. C. Reichardt, *Solvents and Solvent Effects in Organic Chemistry*, 2<sup>nd</sup> ed., VCH, Weinheim, Germany (1988).
3. I.N. Levine, *Physical Chemistry*, 5<sup>th</sup> ed., Tata McGraw-Hill (2002).

**Note:- In the third semester the student shall have to take one of the following two courses (CH-459 and CH-460) as offered by the department.**

#### **CH-459 Physical Chemistry Laboratory-III (Cr. 3)**

1. Investigation of conductivity of different electrolyte solutions in various media.
2. Determination of partial molal volumes and excess molar volumes for binary and ternary systems.
3. Polarimetric determination of specific rate constant for inversion of sucrose and determination of activation energy.
4. To determine the composition of complex ion in solution by spectrophotometric

method (Job's method) for the systems  $\text{Fe}^{3+}$ -salicylic acid,  $\text{Ni}^{2+}$ -ethyldiamine.

5. Effect of mixture composition on the proton NMR spectrum of protic system; investigation of intermolecular interactions.
6. Voltammetric investigations of given compound(s) under variable experimental conditions.
7. Effect of controlled heating on the composition of given solids and monitoring of their IR-spectra.
8. Purification of the given commercial solvent using pertinent methods of separation (distillation, fractional distillation, reflux).
9. Average molar mass determination of a given polymer by viscosity measurement.
10. Determination of conductivity of given electrolytes at infinite dilution at different temperatures and their correlation with the viscosities of medium.
11. Determination of activation energy for the base catalyzed hydrolysis of the given ester and investigation of reaction mechanism at different temperatures (at least three temperatures (20, 30, 40 °C etc.).
12. Study of two phases by mixing water and 1-butanol by refractometer. Spectrometric investigation of the distribution of a given transition metal ion between the two phases.

#### **Recommended Books**

1. A.M. Halpern and G.C. Mcbane, *Experimental Physical Chemistry: A Laboratory Textbook*, Freeman (2006).
2. A.W. Davsion, *Laboratory Manual of Physical Chemistry* (1995).

#### **Supplementary Book**

1. J.A. Beran, *Chemistry in the Laboratory: A Study of Chemical and Physical Changes*, Halsted Pr Publishers (1996).

#### **CH-460 Thesis/Research Project in Physical Chemistry (Cr. 3)**

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

**Note:- In the fourth semester the student shall have to take one of the following two courses (CH-461 and CH-467) as offered by the department.**

#### **CH-461 Advanced Physical Chemistry Laboratory-IV (Cr. 3)**

The course teacher(s) shall offer advanced level practicals involving different experimental facilities available in the section/department. The details of the laboratory work and the equipment involved shall be decided by the teacher concerned on the basis

of the courses taught.

### **CH-467 Thesis/Research Project in Physical Chemistry (Cr. 3)**

The student shall undertake and complete short research project under the supervision of a teacher. The evaluation shall be based on its oral presentation and written report.

### **CH-462 Electrochemistry (Cr. 2)**

**Basic concepts of electrochemistry:** Types of Electrodes and electrochemical cells. **Theories of electrolytes:** Interfacial phenomenon; electrical double layer: Gouy, Stern, Helmholtz models. **Electrode kinetics:** Difference between controlled potential and controlled current techniques; essentials of heterogeneous kinetics, Butler-Volmer's equation, concept and use of exchange current, Tafel's equation and Tafel's plots. **Batteries and fuel cells:** Principle, working and types.

#### **Recommended Books**

1. P.H. Rieger, *Electrochemistry*, 2<sup>nd</sup> ed., Chapman and Hall, New York (1993).
2. A.J. Bard and L.R. Faulkner, *Electrochemical Methods: Fundamentals and Applications*, 2<sup>nd</sup> ed., Wiley (2001).

#### **Supplementary Books**

1. J. O'M Bockris, A.KN. Reddy and M.F. Gombao, *Modern Electrochemistry: Fundamentals of Electrodes*, 2<sup>nd</sup> ed., Springer (2000).
2. V.S. Bagotskii, *Fundamentals of Electrochemistry*, 2<sup>nd</sup> ed., Wiley, New York (2005).

### **CH-463 Polymer Chemistry (Cr. 2)**

**Definition and classification of polymers:** Linear polymer, block copolymers and graft copolymers. **Polymerization and co-polymerization:** Polycondensation polymerization, free radical polymerization, anionic and cationic polymerization. Polymer molecular characterization; number-average and weight-average molar mass. **Characterization techniques:** Gel permeation chromatography, dilute solution viscometry, vapour pressure osmometry, membrane osmometry, ultra-centrifugation, static and dynamic laser light-scattering techniques and polymer rheology. **Structure-property relationship:** Elastomers; plastics; blends and alloys.

#### **Recommended Books**

1. F.W. Billmeyer, *Textbook of Polymer Science*, 3<sup>rd</sup> ed., John Wiley and Sons, Singapore (1994).
2. J.E. Fried, *Polymer Science and Technology*, Prentice-Hall, New Jersey (1995).

#### **Supplementary Books**

1. P. Munk, *Introduction to Macromolecular Science*, Singapore, John Wiley and

Sons, New York (1989).

2. B. Chu, *Laser Light-Scattering, Basic Principle and Practice*, 2<sup>nd</sup> ed., Academic Press, Inc., New York (1991).

#### **CH-464 Surface Chemistry (Cr. 2)**

**Adsorption:** Surface and interface; interfacial tension; adsorption forces, thermodynamics of adsorption; porosity; particle size distribution. Physisorption and chemisorption; adsorption isotherms and their types (Freundlich, Langmuir, BET etc.). Force field in fine pores; microporosity. **Catalysis:** homogeneous and heterogeneous catalysis and gas-solid interface; enzyme catalysis; gas reactions at solid surfaces; diffusion limitations and compensation effect.

#### **Recommended Book**

1. G.C. Bond, *Heterogeneous Catalysis: Principles and Applications*, 2<sup>nd</sup> ed., Clarendon Press, Oxford (1987).

#### **Supplementary Book**

1. S.J. Gregg and K.S.W. Sing, *Adsorption, Surface Area and Porosity*, 2<sup>nd</sup> ed., Academic Press, London (1982).

#### **CH-465 Photochemistry (Cr.2)**

**Fundamentals:** Light and nature of electromagnetic radiations. Electronic structure of atoms; term symbols; absorption and emission of radiations. Interaction of light with atoms and molecules. **Laws of photochemistry:** Photo excited molecules; monophotonic and multiphotonic processes, photodissociation. **Organic and inorganic photochemistry:** Photo-electrochemistry; photochemical reactions in gas phase and in solutions; quantum yield. **Applications:** Photographic, photo-polymerization, drugs and pigments, energy conversions.

#### **Recommended Books**

1. P. Suppan, *Chemistry and Light*, The Royal Society of Chemistry, London (1994).
2. R.P. Wayne, *Principles and Applications of Photochemistry*, Oxford University Press (1988).

#### **Supplementary Books**

1. J.G. Calvert, and J.N. Pitts, *Photochemistry*, John Wiley and Sons Inc., New York (1966).
2. C.E. Wayne, *Photochemistry*, Oxford University Press, London (1996) ISBN: 0198558864.



## CH-466      Colloids and Surfactants (Cr. 2)

**Capillarity:** Surface tension, Young and Laplace and Kelvin equations, orientation at interfaces, thermodynamics of binary systems, the Gibbs adsorption equation. **Surfactants:** Nature and classification, micellization, solubilization, critical micelle concentration, micellar catalysis. **Emulsion:** Emulsion stability, aging and inversion of emulsions, hydrophile-lipophile balance, microemulsions, wetting and contact angle. **Colloidal solutions:** Rheology of dispersions, static and dynamic light-scattering, lyophobic and association colloids, forces in colloidal systems.

### **Recommended Books**

1. A.W. Adamson, *Physical Chemistry of Surfaces*, 5<sup>th</sup> ed. Wiley-Interscience Publication, John Wiley & Sons, Inc., New York (1990).
2. P.C. Hiemenz and Rajagopalan, *Principles of Colloid & Surface Chemistry*, 3<sup>rd</sup> ed. Marcel Dekker Inc., New York (1997).
3. M.J. Rosen, *Surfactants and Interfacial Phenomena*, Wiley-Interscience Publication, John Wiley & Sons, New York (1978).

### **Supplementary Book**

1. D.F. Evans and H. Wennerström, *The Colloidal Domain Where Physics, Chemistry, Biology and Technology Meet*, VCH Publishers, Inc., New York (1994).

## 3<sup>rd</sup> Semester (Compulsory Course)

### CH-360      Environmental Chemistry (Cr. 3)

**Introduction:** Environmental Chemistry, Environmental segments, Species present in Environment, Types of Pollution, Environmental radioactivity. **Atmospheric pollution:** The atmosphere, composition, temperature and pressure profile, role of free radicals in the atmosphere, temperature inversion and photochemical smog, particulate matter in the atmosphere, Industrial pollutants, atmospheric aerosols, acid-rain major sources, mechanism, control measures and effects on buildings and vegetation, global warming, major greenhouse gases, mechanism, control measures and global impact, the stratospheric ozone—the ozone hole, CFCs, ozone protection, biological consequences of ozone depletion. **Water Pollution:** Water pollution and waste water treatment, municipal, industrial and agricultural sources of pollution, heavy metals contamination of water, eutrophication, detergents and phosphates in water, water quality criteria, water purification: primary, secondary and advanced treatment, removal of nitrogen and phosphorous compounds from polluted water, organic matter in water and its decomposition. **Land pollution:** Soil and mineral resources, general principles of metal extraction, heavy metals contamination of soil, toxicity of heavy metals, bio-accumulation of heavy metals, organic matter in soil, macro and micro-nutrients in soil, ion-exchange in soil, soil pH and nutrients availability. **Solid pollutants:** Classification and origin of solid wastes, Characteristics of solid wastes, Solid waste treatment and methods of disposal. **Toxic and Hazardous Waste:** Types of toxic and hazardous waste, Radioactive waste, Nuclear waste management, Toxic chemicals, Treatment and disposal

of hazardous waste, Control and treatment of trace elements. **Green Chemistry:** Atom economy, integrated pests management control (IPMC), ionic liquids, super critical extraction technology, green synthesis, recycling, carbon dioxide sequestering, water based paints.

### Recommended Books

1. C. Baird, M. Cann, *Environmental Chemistry*, 5<sup>th</sup> ed., W.H. Freeman & Company, (2012).
2. S.S. Dara and D.D. Mishra, *A Text Book of Environmental Chemistry and Pollution Control*, 9<sup>th</sup> ed., S. Chand & Co. Ltd., (2004).
3. R. Singhi and V. Singh, *Green Chemistry for Environmental Remediation*, John-Willey & Sons, Inc., (2011).
4. A.M. Holloway and R.P. Wayne, *Atmospheric Chemistry*, 1<sup>st</sup> ed., Royal Society of Chemistry, (2010).
5. M. Vaclavikova, K. Vitale, G.P. Gallios and L. Ivanicova, *Water Treatment Technologies for Removal of High Toxicity Pollutants*, Springerlink, UK, (2010).
6. S.E. Manahan, *Environmental Chemistry*, 9<sup>th</sup> ed., CRC press, Taylor & Francis group, USA, (2009).
7. J.E. Girard, *Principles of Environmental Chemistry*, 2<sup>nd</sup> ed., Jones and Bartlett publishers, (2010).
8. R.M. Harrison, P. Monks, J.G. Farmer, M.C. Graham, S.J. Mora, I. Pulford, and C. Hulsal, *Principles of Environmental Chemistry*, 1<sup>st</sup> ed., Royal Society of Chemistry, (2007).
9. A. Matalack, *Introduction to Green Chemistry*, 2<sup>nd</sup> ed., CRC press, Taylor & Francis group, USA, (2010).
10. J. Wright, *Environmental Chemistry*, Routledge, (2003).
11. P. O'Neill, *Environmental Chemistry*, 3<sup>rd</sup> ed., Blackie Academic & Professional, (1998).
12. D.M. Elsom, *Atmospheric Pollution: A Global Problem*, 2<sup>nd</sup> ed., Wiley-Blackwell, (1992).

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