# B.Sc. 6<sup>th</sup> SEMESTER DISCIPLINE SPECIFIC ELECTIVES (DSEs) <u>OPTION-I</u>

#### CH620DA: CHEMISTRY: SPECTROSCOPY

**Course Weightage: 04 Credit (Theory)** 

#### Course Objectives:

*To provide basic knowledge of spectroscopy and its applications. Course outcomes: The students after learning the course will be able to understand;* 

- 1. The regions of electromagnetic spectrum and its interactions with matter.
- 2. The underlying principles involved in transitions (rotational, vibrational, electronic NMR), interpretation of the corresponding spectra and applications

# THEORY: 4 CREDITS

Unit- I Spectroscopy-I

*Spectroscopy*: Electromagnetic radiation, regions of the spectrum, Representation of molecular spectrum, Peak position, intensity and width. Types of peak broadening. Statement of Born-Oppenheimer approximation.

**Rotational spectrum:** Moment of inertia, classification of molecules on the basis of moment of inertia. Energy of a rigid diatomic rotor, selection rules for rotational transition and associated spectrum, relative population of rotational levels and spectral intensity, determination of bond length in diatomic molecules.

# Unit-II Spectroscopy-II

*Vibrational Spectrum:* Classical and quantum mechanical (qualitative) treatment of simple harmonic oscillator, selection rules for vibrational transition, pure vibrational spectrum of a diatomic molecule, determination and relation of force constant with bond length and bond energy.

Molecular vibrations, IR transitions and selection rules. Group frequency and fingerprint regions and its significance. Effect of resonance, inductive effect and H-bonding on infrared absorptions. Characteristic absorptions of alkanes, alkenes, alkynes, alcohols, ethers, carbonyl compounds, amines and carboxylic acids and their derivatives.

# Unit- III Spectroscopy-III

*Photochemistry:* Laws of photochemistry. Grothus-Drapper law, Stark-Einstein law. Beer-Lambert law, molar absorptivity. Jablonski diagram-fluorescence, phosphorescence, non-radiative processes (internal conversion, intersystem crossing) quantum yield.

*Ultraviolet-visible spectroscopy:* Presentation and analysis of electronic spectra. Types of electronic excitations. Chromophores and auxochromes. Bathochromic and hypsochromic shifts. Effects of conjugation and solvents on absorption bands. Ultraviolet spectra of enes and enones. Prediction of maxima of enes using Woodward's rules.

# o understand;

No. of Contact Hours: 60

Max. Marks: 60

# rations

# (15 Contact hours)

# (15 Contact hours)

(15 Contact hours)

# Unit- IV Spectroscopy-IV

# (15 Contact hours)

*Nuclear Magnetic Resonance Spectroscopy:* Basic principles of NMR spectroscopy. Shielding and deshielding of protons. The chemical shift. Equivalent and non-equivalent protons. Spin-spin splitting, coupling constants for vicinal, geminal and long-range couplings. Characteristic functional group NMR absorptions. The <sup>1</sup>HNMR spectra of ethyl bromide, ethanol, acetaldehyde, ethyl acetate, methyl propionate, toluene and acetophenone.

- 1. Fundamentals of Molecular Spectroscopy; C. N. Banwell, E.M. McCash; 4<sup>th</sup>Edn. (Indian Edn.), Tata McGraw-Hill, 2017.
- 2. Principles of Physical Chemistry; B.R. Puri, L.R. Sharma and L.S. Pathania; 47<sup>th</sup>Edn. Vishal Pubs & Co, 2017.
- 3. Spectroscopy of Organic Compounds; P.S. Kalsi; 7<sup>th</sup>Edn, New Age International Pvt. Ltd., 2016.
- 4. Introduction to Spectroscopy; D.L. Pavia, G.M. Lampman, G.S. Kriz, J.R Vyvyan;5<sup>th</sup>Edn., Cengage Learning India Pvt. Ltd., 2015.
- 5. Organic Spectroscopy; L.D.S. Yadav; 1<sup>st</sup> Edn, Springer Netherlands, 2005.
- 6. Organic Spectroscopy; W. Kemp; 3<sup>rd</sup>Edn, Palgrave Macmillan, 2008.
- 7. Kakkar, R. Atomic & Molecular Spectroscopy: Concepts & Applications, Cambridge University Press; 2015.
- 8. John R. Dyer: Applications of Absorption Spectroscopy of Organic Compounds, Prentice Hall.
- Spectrometric Identification of Organic Compounds; R. M. Silverstein, F. X. Webster, D. J. Kiemle, D. L. Bryce; 8<sup>th</sup>Edn., John Wiley & Sons, 2014.

#### B.Sc. 6<sup>th</sup> SEMESTER-CHEMISTRY LAB COURSE (OPTION-I)

# CH620DA: PRACTICALS

### Max. Marks: 30

#### **Course Weightage: 02 Credit**

#### No. of Contact Hours: 60

### Part 1: Spectrophotometry

- 1. To determine the  $\lambda_{max}$  of KMnO<sub>4</sub> and K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> and calculate the energies of two absorption bands in these molecules in different units.
- 2. Verify Lambert-Beer's law
- 3. Determination of unknown concentration of CuSO<sub>4</sub>/KMnO<sub>4</sub>/K<sub>2</sub>Cr<sub>2</sub>O<sub>7</sub> in a solution using spectrophotometer.
- 4. Spectrophotometric determination of Fe (II), using 1, 10-Phenanthroline.

#### Part 11: Refractometry

- 1. To determine refractive index of a liquid by using Abbe's refractometer.
- 2. To determine percentage composition of a mixture of two liquids by refractometry (Glycerol and water).

- 1. Advanced Practical Physical Chemistry; J.B. Yadav; Krishna Prakashan Media (P) Limited, 2015.
- 2. Senior Practical Physical Chemistry PB; B. D. Khosla; V. C. Garg; A. R. Gulati; R. Chand & Co, 2008.
- 3. Vogel's Qualitative Inorganic Analysis; G. Svehla; 7th Ed., Pearson Education. 2013.
- 4. Vogel's Textbook of Quantitative Inorganic Analysis; Bassett, G. H. Jeffery, J. Basset, J. Mendham, R. C. Denny, 6th ed., ELBS; 2007.
- 5. Experimental Physical Chemistry; A. M. Halpern, & G. C. Mc Bane; 3rd Ed.; W.H. Freeman & Co; 2006.
- 6. Experiments in Physical Chemistry; C. W.; Garland, J. W. Nibler, & D. P. Shoemaker, 8th Ed.; McGraw-Hill: New York, 2003.
- 7. Principles of Instrumental Analysis; D.A. Skoog, F.J. Holler & T.A. Nieman Cengage Learning India Ed.

# B.Sc. 6<sup>th</sup> SEMESTER DISCIPLINE SPECIFIC ELECTIVES (DSEs)

# **OPTION-II**

# CH620DB: CHEMISTRY: ENVIRONMENTAL AND GREEN CHEMISTRY

# **Course Weightage: 04 Credit (Theory)**

Max. Marks: 60 No. of Contact Hours: 60

#### Course Objectives:

To sensitize students about importance of environment and ways to keep it pollution free.

#### Course outcomes: The students after learning the course will be able to understand:

- 1. The harmful impacts of chemicals on the environment.
- 2. The design of a green process/reaction in lab.
- 3. The synthesis of industrially important chemicals using green approach.

# UNIT I: Environmental Chemistry-I

Physical characteristics of atmosphere, Stratification of atmosphere, Energy and mass transfer in the atmosphere, Chemical and photochemical reactions in the atmosphere, Acid-base reactions in the atmosphere, Organic and inorganic particulate matter in the atmosphere, Atmospheric pollutant gases, Acid rain, formation of acid rain and its effects, Photochemical smog: Formation and effects, Greenhouse gases and global warming, Ozone layer depletion.

**Soil:** Nature and composition of soil, Inorganic and organic matter of soil, soil humus, Soil solution, Acid-base and ion exchange reactions in soils, Macronutrients in soil, N, P, K in soil, Micronutrients in soil.

# UNIT II: Environmental Chemistry-II

Wastes and pollutants in soil, soil pH, acidity, alkalinity, Influence of pH on soils, redox potential and reduction processes in soils, chemical reactions in soil (reactions in soil solution, ion-exchange, ligand exchange, complexation and precipitation).

Introduction to aquatic chemistry: Gases in water, Nature and types of pollutants in water, Elemental pollutants, Heavy metals, metalloids, Inorganic pollutants, Algal nutrients and eutrophication, acidity, alkalinity and salinity, BOD, organic pollutants (sewage, soaps and detergents), pesticides in water, water disinfection, water reuse and recycle.

# UNIT 1II: Green Chemistry-I

Need for green chemistry and role of chemists. Green chemistry and its 12 basic principles (detailed overview of principles along with examples). Planning a green synthesis in a laboratory (choice of starting materials, reagents, catalysts, solvents, reaction-conditions like energy sources).

Green solvents: Water, ionic liquids, supercritical water and carbon dioxide.

Green catalysts: Acid, base and oxidation catalysts, biocatalysts, phase transfer catalysis

# (15 contact hours)

# (15 Contact hours)

(15 contact hours)

# UNIT IV: Green Chemistry-II

#### (15 Contact hours)

*Green reactions in Solid phase/Ionic liquids:* Aldol condensation, Cannizaro, Claisen-Schmidt and Grignard reactions.

Phase-Transfer Catalysis: Michael-addition and Williamson's ether synthesis.

*Enzymatic Transformations:* Benzoin condensation, Reduction of aldehydes/ketones using Baker's yeast/*Daucus carota*.

*Green processes of Industrial importance:* Synthesis of styrene, adipic acid, catechol, urethane, caprolactam, paracetamol, ibuprofen, slidenafilcitrate, (*S*)-metachlor, citral, vanillin, menthol and bioethanol using green route and comparision with their conventional synthetic routes.

- 1. New Trends in Green Chemistry, V. K. Ahluwalia, M. Kidwai: Anamaya Publishers: New Delhi: Ist Edition: 2004.
- 2. Green Chemistry-Environment Friendly Alternatives, RashmiSanghi& M. M. Srivastava: Narosa: 2007.
- 3. Green Chemistry-An Introductory Text; IInd Edition: Mike Lancaster: RSC: 2010.
- 4. Green Chemistry-Theory and Practice; P.T. Anastas and J. C. Warner; Oxford; 2000
- 5. Green Chemistry-Environmentally Benign Reactions, V.K. Ahluwalia, Anne Books Pvt. Limited; 2012.
- 6. Green Chemistry: Fundamentals and applications, S.C. Ameta, R.Ameta, Apple academic press, 2013.
- 7. Green Chemistry and Processes: MukeshDoble, Anil Kumar Kruthiventi; Academic Press-Elsevier 2007.
- 8. Principles of Environmental Chemistry, R. M. Harrison: RSC Publishing, 2007.
- 9. Environmental Chemistry, S. E. Manahan, CRC Press LLC, 2000.
- 10. Environmental Chemistry; A. K. De, 7th Edn; New Age International Pvt Ltd; 2010.
- 11. Environmental Chemistry Fundamentals, J.G. Ibanez, M.H. Esparza, C.D. Serrano, A.F. Infante, M. M Singh, Springer Publishers, 2007.

### B.Sc. 6<sup>th</sup> SEMESTER-CHEMISTRY OPTION-II (LAB COURSE)

# CH620DB: PRACTICALS Course Weightage: 02 Credit

# Max. Marks: 30 No. of Contact hours: 60

# Part 1: Green Chemistry

- 1. Micelle assisted reduction of aromatic carbonyl compound in water using NaBH<sub>4</sub> (Aqueous phase reaction)
- 2. Photoreduction of benzophenone to benzopinacol in presence of sunlight (Photochemical reaction).
- 3. Reduction of acetophenone using *Daucuscarrota*root (Enzymatic transformations).
- 4. Aldol condensation in solid phase between an aromatic aldehyde and acetophenone(Solid phase reaction).
- 5. Solid phase synthesis of hydrazone from an aromatic aldehyde/ketone and phenyl hydrazine.

# Part-II: Environmental Chemistry

- 1. Determination of pH of soil sample using pH meter.
- 2. Determination of pH, acidity and alkalinity of a water sample.
- 3. Determination of total soluble salts in soil using conductance measurements.
- 4. Determination of carbonate and bicarbonates in soil.
- 5. Estimation of total hardness of water by EDTA method.
- 6. Determination of calcium, magnesium and iron in soil.
- 7. Determination of dissolved oxygen (DO) of a water sample.
- 8. To determine the total residual chlorine in a water sample.
- 9. To determine chloride ion in a given water supply by argentometric method.

- 1. Green Chemistry: Environmentally Benign Reactions, V.K. Ahluwalia 2<sup>nd</sup> Edition, Ane Books Pvt. Ltd, 2012.
- 2. Green Chemistry Experiment: A monograph International Publishing House Pvt Ltd. New Delhi. Bangalore Sharma, R.K.; Sidhwani, I.T. &Chaudhari, M.K. I.K. (2013).
- 3. Solvent Free Organic Synthesis, Koichi Tanaka; Wiley VCH VerlagGmbHand Co. KGaWienhiem Germany.
- 4. Introduction to Organic Laboratory Techniques: A Microscale and Macro Scale Approach, Pavia, D.L., Lampman, G.M., Kriz, G.S. & Engel, R.G. 1995.
- 5. A Laboratory Manual for Environmental Chemistry, R. Gopalan, R. W. Sugumar, I K International Publishing house Pvt. Ltd; 2008.
- 6. Experiments in Environmental Chemistry: A laboratory Manual, D. W. Connell and P.D. Vowles, IstEdn., Pergamon International Library, 1980.
- 7. Quantitative Chemical Analysis, D. C. Harris, 8<sup>th</sup>Edn. W. H. Freeman. And Co, 2010.