**Programme: M. Sc. Part-I (Chemistry)**

**Course Code: ACC-401** **Title of the Course: Concepts in Analytical Spectroscopy**

**Number of Credits: 03** **Effective from AY: 2018-19**

| | | |
|---|---|---|
| **Prerequisites for the course:** | Students should have studied the spectroscopic techniques such as UV-Vis, IR at FY B Sc, S Y B Sc or T Y B Sc levels so as to have basic knowledge of spectroscopy and basic principles. | |
| **Course Objectives:** | 1. Introduction of various concepts in molecular and atomic spectroscopy.<br>2. Learning data analysis, handling and interpretation of spectra | |
| **Course Outcomes:** | 1. Students should be in a position to use spectroscopic methods for qualitative and quantitative analysis.<br>2. Evaluate the utility of UV/Vis spectroscopy as a qualitative and quantitative method.<br>3. Identification of functional group based on IR spectra<br>4. Students should be in a position to predict the structure based on IR, NMR, MS data. | |
| **Content:** | **1.Introduction to spectrochemical methods**<br>1.1. Interaction of Electromagnetic Radiation with Matter: electromagnetic spectra, Regions of Spectrum; Numericals.<br>1.2 Electronic spectra and Molecular structure: kinds of transition, Chromophores and auxochrome; absorption by isolated chromophores, conjugated chromophores, aromatic compounds, inorganic chelates.<br>1.3. Infrared absorption and molecular structures: IR spectra, overtones and bands-basis of NIR absorption<br>1.4. Spectral Databases: Identification of unknown; Application of UV-Vis and IR spectroscopy for identification of unknown compounds<br>1.5. Solvents for spectrometry: Choices and effect of solvents on UV-Vis and IR spectra.<br>1.6. Quantitative Calculations: The Lambert-Beer's Law; Mixtures of absorbing species-laws of additivity of absorbance; calibration curve for calculation of unknown; Spectrometric errors in measurement; Deviation from Lambert-Beer's law-chemical deviation, instrumental deviation; Quantitative measurement from IR spectra; Numericals for quantitative analysis using UV-VIS spectroscopy.<br>1.7. Spectrometric Instrumentation of UV-Vis and IR (brief introduction only): Sources, monochromators, sample cells, Types of instruments; detectors; Instrumental wavelength and absorption calibration.<br>(Chapter 16: Analytical Chemistry, G.D. Christian, 6$^{th}$Ed.)<br><br>**2. Molecular Luminescence: Fluorimetry, Phosphorimetry and Raman Spectroscopy**<br>2.1. Introduction,<br>2.2. Fluorimetry : Theory and basic principle; Quenching; Spectrofluorimeters and applications<br>2.3. Phosphorimetry: Theory and basic principle; phosphorimeters and application<br>2.4. Raman Spectroscopy: Theory and Structural analysis using Raman Spectra<br>(Chapter 6: Instrumental Methods of Chemical Analysis, G.W. Ewing,5$^{th}$Ed)<br>**3. Atomic Spectroscopy**<br>3.1. Principles of emission<br>3.2. Atomic Emission spectroscopy (AES)<br>3.3. Flame Emission spectroscopy (FES) | 12 hr<br><br>4 hr<br><br>6 hr |

| | | |
|---|---|---|
| | 3.4. Atomic absorption Spectroscopy (AAS)<br>3.5. X-Ray Fluorescence Spectroscopy (XRF)<br>(Introduction, principles and applications of above techniques shall be discussed; Chapter 13: Analytical Chemistry Principles, J.H. Kennedy, 2nd ed)<br><br>**4.Spectrometric Identification of Organic compounds**<br>**4.1 Ultraviolet and visible Spectroscopy :** Brief Revision of UV/VIS Spectroscopy **;**Instrumentation and Sampling ; Applications of Electronic S pectroscopy:Conjugated Dienes, Trienes, polyenes, a, ßunsaturated carbony l compounds, aromatic hydrocarbons (Assignment based on BSc. Syllabus for calculating λmax) (Kemp – Chap4)<br>**4.2 Infrared Spectroscopy:** Introduction to IR spectroscopy; Basic IR spectra interpretation; Frequencies of functional group. (Kemp – Chap2).<br>**4.3 Proton and Carbon NMR Spectroscopy:** Theory of NMR **;** Chemical shift; factors influencing chemical shift **;** Solvents used in NMR; Theory of spin-spin splitting and simple spin systems;Coupling constant calculation; Factors influencing coupling constant (Assignment based on BSc. Syllabus) (Kemp - Chapter 3)<br>**4.4 Mass Spectrometry :** Basic PrinciplesandInstrumentation: Problem solving in structure elucidation based on MS (Kemp - Chapter 5)<br>**4.5. Conjoint Spectrometry Problems:** Structural elucidation of organic molecules using UV, IR, NMR ($^{1}H$,$^{13}C$), MS, (Silverstein)<br><br>(**Note:**Assignment based on BSc. syllabus for all above spectrometric structure should be given to student. *More weightage of lectures shall be given for solving IR and NMR data for structur elucidation*) | 14 hr |
| **Pedagogy:** | Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. Sessions shall be interactive in nature to enable peer group learning. | |
| **Text Books References / Readings** | 1. G. D. Christian; *Analytical Chemistry*, John Wiley; 6th Edition.<br>2. J.H. Kennedy, *Analytical Chemistry: Principles*, Saunders College Publishing, 2nd Edition.<br>3. G. W. Ewing, *Instrumental Methods of Chemical Analysis*, McGraw-Hill Int 5th Ed.<br>4. W. Kemp; *Organic Spectroscopy*; Palgrave; 3 Ed.<br>5. D.A. Skoog, D.M. West, F.J. Hollar, S.R. Crouch; *Fundamentals of Analytical Chemistry*, Cengage learning; 9 Ed.<br>6. J. Mendham, R.C. Denney, J.D. Barnes and M. Thomas; *Vogel's Textbook of Quantitative Inorganic Analysis;* 6th Edition, Pearson Education Asia 2005<br>7. H. Willard, L.L. Merritt, J.A. Dean, F.A. Settle, *Instrumental methods of Analysis*; HCBS Publishing New Delhi; 2004, 7th Ed.<br>8. C.N. Banwell and E.M. McCash, *Fundamentals of Molecular Spectroscopy*, Tata McGraw- Hill, New Delhi; 4th Ed.<br>9. R. M. Silverstein, F.X. Webster; *Spectrometric identification of Organic Compounds*; Wiley- India; 6th Ed.<br>10. H. Gunzler & A. Williams; *Handbook of Analytical Techniques*, WILEY-VCH Verlag GmbH; 2001, 1st Ed.<br>11. P.S. Kalsi; *Spectroscopy of Organic Compounds*; New Age Internationa l; 2 Ed.<br>12. R.T. Morrison, R.N. Boyd; *Organic Chemistry*, Prentice Hall India 4th Edition<br>13. E. Pretsch, P. Buhlmann, C. Affolter; *Structural Determination of Organic Compounds*, Springer; 2005; 2nd Ed. | |