

GOVERNMENT COLLEGE (AUTONOMOUS), RAJAMAHENDRAVARAM

DEPARTMENT OF CHEMISTRY

CBCS Syllabus for B.Sc. III Year

Effective from 2018 – 2019 onwards

Paper - VIII-C-1 Semester – VI

ORGANIC SPECTROSCOPIC TECHNIQUES

Course Code: CHE120

No. of h/w : 3

UNIT-I

10 h

Nuclear Magnetic Resonance Spectroscopy

Nuclear spin, Principles of NMR - Classical and Quantum Mechanical methods, Magnetic moment and Spin angular momentum. Larmour Frequency. Instrumentation. Relaxation - spin-spin & spin lattice relaxation. Shielding constants, Chemical shifts, Shielding and Deshielding mechanism - Factors influencing Chemical shift. Spin-Spin interactions - AX, AX₂ and AB types. Vicinal, Geminal and Long range coupling - Factors influencing coupling constants.

UNIT – II

5 h

Spin decoupling, Spin tickling, Deuterium exchange, Chemical shift reagents and Nuclear Overhauser effect. Applications in Medical diagnostics, Reaction kinetics and mechanically induced dynamic nuclear polarization. FT NMR and its advantages.

UNIT-III

10 h

UV & Visible Spectroscopy

Electronic spectra of diatomic molecules. The Born-oppenheimer approximation. Vibrational coarse structure: Bond association and Bond sequence. Intensity of Vibrational - electronic spectra: The Franck-Condon principle. Rotational fine structure of electronic vibration transitions. Electronic structure of diatomic molecules.

Types of transitions, Chromophores, Conjugated dienes, trienes and polyenes, unsaturated carbonyl compounds – Woodward-Fieser rules.

UNIT-IV**5 h**

Electronic spectra of polyatomic molecules. Chemical analysis by Electronic Spectroscopy – Beer- Lambert's Law. Deviation from Beer's law. Quantitative determination of metal ions (Mn^{+2} , Fe^{+2} , NO_2^- , Pb^{+2}). Simultaneous determination of Chromium and Manganese in a mixture.

UNIT-V**15 h****Electron Spin Resonance Spectroscopy**

Basic Principles, Theory of ESR, Comparison of NMR & ESR. Instrumentation, Factors affecting the 'g' value, determination of 'g' value. Isotropic and Anisotropic constants. Splitting hyper fine splitting coupling constants. Line width, Zero field splitting and Kramer degeneracy. Crystal field splitting, Crystal field effects.

Applications:- Detection of free radicals - ESR spectra of Methyl radical (CH_3^\bullet), Benzene anion ($C_6H_6^-$), Isoquinine, $[Cu(H_2O)_6]^{+2}$ and $[Fe(CN)_5NO]^{-3}$

REFERENCE BOOKS

1. Electron Spin Resonance Elementary Theory and Practical Applications - John E. Wertz and James R. Bolton, Chapman and Hall, 1986.
2. Spectroscopic Identification of organic compounds – Silverstein, Basseler and Morrill.
3. Organic Spectroscopy - William Kemp.
4. Fundamentals of Molecular Spectroscopy - C.N.Banwell and E.A. Mc cash 4th Edition, Tata Mc Graw Hill Publishing Co., Ltd. 1994.
5. Physical Methods in Inorganic Chemistry – R.S.Drago, Saunders Publications.
6. Application of Mössbauer Spectroscopy – Green Mood.
7. NMR, NQR, EPR and Mössbauer Spectroscopy in inorganic chemistry – R.V.Parish, Ellis, Harwood.
8. Instrumental Methods of Chemical Analysis - H.Kaur, Pragathi Prakashan, 2003.

9. Instrumental Methods of Analysis, 7th Edition – Willard, Merrit, Dean, Settle, CBS Publications, 1986.
10. Molecular Structure and Spectroscopy – G.Aruldas, Prentice Hall of India Pvt.Ltd, New Delhi, 2001.
11. Mössbauer Spectroscopy – N.N.Green Wood and T.C.Gibb, Chapman and Hall, Landon 1971.
12. Coordination Chemistry: Experimental Methods - K.Burger, London Butter Worths, 1973.
13. Analytical spectroscopy – Kamlesh Bansal, Campus books, 2008.
14. Structural Inorganic Chemistry Mossbauer Spectroscopy – Bhide.
15. Principle of Mössbauer Spectroscopy – T.C.Gibb, Chapman and Hall, Landon 1976.