CH 408: MOLECULAR SPECTROSCOPY (3-1-0: 4)

Introduction

Electromagnetic radiation, interaction of electromagnetic radiation with matter, natural line width and natural line broadening, intensity of spectral lines, time dependent perturbation theory, Born-Oppenheimer approximation.

Rotational and vibrational spectra

Classification of molecules according to their moments of inertia, rotational energy levels, selection rule, intensity of spectral lines, effect of substitution in microwave spectra, stark effect, spectra of symmetric top and asymmetric top type molecules.

Linear harmonic oscillator, vibrational energy levels of diatomic molecules, anharmonicity, potential energy diagram, vibration–rotational spectra of diatomic molecules, polyatomic molecules (CO_2, NH_3 etc.) selection rules, fundamental, overtone and combination bands, hot bands, group frequencies, factors affecting the band positions and intensities, far I.R. regions, brief description of instrumental techniques.

Theories of Raman Effect, condition for Raman active vibrations, selection rules, mutual exclusion principle, rotational Raman spectra, vibration–rotation Raman spectra.

Electronic spectra

Born-Oppenheimer approximation, Frank-Condon principle, ground and excited states of diatomic molecules, selection rules for electronic transitions; Fluorescence, phosphorescence and Chemiluminescence; electronic spectra of polyatomic molecule, Beer-Lambert's law, chromophores, auxochromes, solvent effect, calculation of absorption maxima by Woodward-Fieser Rules.

Nuclear magnetic resonance spectroscopy

Basic principles of NMR spectroscopy, chemical shifts, factors affecting the chemical shifts, spin-spin coupling, coupling constant, spin – spin interaction between different interacting nuclei (first order spectra), relaxation processes, nuclear magnetic double resonance, nuclear Overhouser effect (NOE), two dimensional NMR, NOESY, DEPT, INEPT spectra, shift reagents, instrumentation, FT NMR and introduction to MRI and solid state NMR.

EPR spectroscopy

Basic principles, origin of g-shifts, isotropic and anisotropic hyperfine coupling, zero field splitting, Kramer degeneracy, ESR analysis of some organic compounds, transition metal complexes.

Mass spectrometry

Basic principles and instrumentation; ionization techniques, molecular ion peak, isotopic peaks, metastable peak, recognition of molecular ion peak, fragmentations patterns – general rules, structure elucidation of organic compounds.

Mössbauer spectroscopy

Nuclear resonance absorption, recoil energy, Doppler Effect, Mössbauer effect, isomer shifts, quadrupole splitting, effect of magnetic field, applications to iron, tin and cobalt compounds.

Text Books and References

1. C. N. Banwell and E. M. McCash, "Fundamentals of Molecular Spectroscopy", Tata McGraw Hills
2. D. Pavia, G. Lampman, G. Kriz and J. Vyvyan, "Introduction to Spectroscopy", Brooks Cole.

3. R. M. Silverstein, F. X. Webster and D. J. Kiemle, “Spectrometric Identification of Organic Compounds”, John Wiley & Sons.
4. W. Kemp, “Organic Spectroscopy”, Palgrave Macmillan.