



# MOLECULAR SPECTROSCOPY: A PHYSICAL CHEMIST'S PERSPECTIVE

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**INTENDED AUDIENCE :** Chemistry, Physics and UG students of Engineering

### COURSE OUTLINE :

This is a comprehensive course on molecular spectroscopy. We start with dispersive and Fourier transform spectroscopic techniques, go on to derive selection rules from Time dependent perturbation theory, develop a quantum mechanical treatment of spin resonance spectroscopy and then move on to a discussion of spectra of polyatomic molecules using symmetry. This course is the same as CH 442 of IIT Bombay

### ABOUT INSTRUCTOR :

Prof. Anindya Datta is a Professor of Chemistry in IIT Bombay, with research interest in ultrafast spectroscopy and time resolved fluorescence microscopy. He has been teaching experience of 17 years. 14 Ph. D. students have graduated from our laboratory. Eight more are working towards their degree. He received Excellence in Teaching Award from our institute in 2017 and have taught two NPTEL courses: one on Molecular Spectroscopy and another on Symmetry in Chemistry.

### COURSE PLAN :

**Week 1 :** Introduction, Dispersive spectrometers, Fourier Transform spectrometers, Signal to Noise Ratio, Microwave Spectroscopy of diatomic molecules

**Week 2 :** Derivation of selection rules for microwave spectra, Simple harmonic oscillator, Selection rule, Rovibrational spectra

**Week 3 :** Anharmonic perturbation, Raman effect, Raman spectroscopy

**Week 4 :** Time dependent perturbation theory, Interaction of radiation with matter, Fermi's golden rule

**Week 5 :** Einstein treatment, Lasers and lineshapes, Laser spectroscopy

**Week 6 :** Magnetic resonance, Classical treatment of relaxation, Pulse sequences

**Week 7 :** Perturbation theory for weak coupling, Variation method for strong coupling, Double resonance techniques

**Week 8 :** Nuclear quadrupole resonance, Zeeman effect, Field effect on diatomic vibrator

**Week 9 :** Hyperfine interactions, Electronic spectra of diatomic molecules, Fortrat diagram

**Week 10 :** Matrix vector formulation of vibration of polyatomic molecules, Normal modes of vibration, Symmetry of normal modes and IR/Raman activity

**Week 11 :** Summary

**Week 12 :** Revision