



# FUNDAMENTALS OF SPECTROSCOPY

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**INTENDED AUDIENCE :** Interested Learners

**INDUSTRY SUPPORT :** It is a basic course. Therefore it is not directly relevant for industrial application

### COURSE OUTLINE :

Spectroscopy is the study of the interaction of light (electromagnetic radiation) with matter. Electromagnetic radiation covers a wide range of frequencies from gamma rays to radio frequencies. Depending on the frequency of radiation interacting with the matter, one can have different forms of spectroscopy. These spectroscopic techniques allow us to monitor the structural properties of matter. For example, information on moment of inertia (and hence bond length) can be obtained from rotational spectrum. Similarly, vibrational spectrum provides information on the force constant, i.e. the strength of a chemical bond. Besides providing information on molecular structure, spectroscopic techniques can also be used for quantitative estimation of a substance making spectroscopy an important analytical tool. Further, a spectroscopic transition is characterized by a definite timescale and this can provide information on molecular dynamics. In this course, the fundamental principles of the different forms of spectroscopy will be elaborated in a unified way from both theoretical and experimental viewpoints. Application of these different spectroscopic methods for the elucidation of molecular structure will also be discussed. The structural and dynamic aspects of spectroscopy are fundamental to physics, chemistry and biology. Thus, this course will provide a thorough conceptual understanding for these branches of science.

### ABOUT INSTRUCTOR :

Prof. SSayan Bagchi: Sayan Bagchi did his B. Sc from Presidency College, Kolkata in 2000. He completed his M. Sc from Indian Institute of Technology, Kanpur. He then joined University of Pennsylvania, Philadelphia, USA in 2002 and completed his Ph. D. in 2008 under the supervision of Professor Robin Hochstrasser. Dr. Bagchi then moved to Stanford University as a postdoctoral researcher. He then joined NCL Pune as a senior scientist and assistant professor (AcSIR) in December, 2012. Dr. Bagchi works on understanding the roles of interactions and dynamics in molecular systems using novel spectroscopic techniques. He also collaborates with theoretical colleagues in various projects to understand the molecular origin of the spectroscopically studied processes. He has over 6 years of teaching experience in spectroscopy..

Prof. Anirban Hazra: Anirban Hazra obtained his integrated M.Sc. from IIT Bombay in 1999. He then joined Princeton University for Ph.D. in theoretical chemistry and submitted his thesis titled "Electronic absorption spectra from first principles". He went for postdoctoral research at Pennsylvania State University. He then joined IISER Pune as an assistant professor in 2011. He became associate professor in 2018. Dr. Hazra's research is primarily on understanding excited state phenomena in molecules. In electronic excited states, unlike in the ground state, the chemistry is largely governed by the crossing of potential energy surfaces or more generally by the coupling of multiple electronic states via nuclear motion. There is a breakdown of the Born-Oppenheimer approximation. Using theoretical methods like multi-reference electronic structure calculations and mixed-quantum classical nuclear dynamics, his group is interested in mechanistic description of the chemistry in these situations.

### COURSE PLAN :

**Week 1:** Origin of a spectrum

**Week 2:** Different Forms of Spectroscopy

**Week 3:** Rotational Spectroscopy

**Week 4:** Rotational Spectroscopy(continued)

**Week 5:** Vibrational Spectroscopy

**Week 6:** Vibrational Spectroscopy(continued)

**Week 7:** Raman Spectroscopy

**Week 8:** Raman Spectroscopy(continued)

**Week 9:** Electronic Spectroscopy

**Week 10:** Electronic Spectroscopy(continued)

**Week 11:** Electronic Spectroscopy(continued)

**Week 12:** Combination of different spectroscopic methods to solve complex problems