



QUANTUM MECHANICS AND MOLECULAR SPECTROSCOPY

PROF. G NARESH PATWARI

Department of Chemistry
IIT Bombay

PRE-REQUISITES : Basic understanding of Quantum Mechanics / Quantum Chemistry.

INTENDED AUDIENCE : Core course for MSc / Elective for PhD

COURSE OUTLINE :

This course is based on application of quantum mechanics to molecular systems to probe their energy levels. Prior understanding of solutions to the time-independent Schrodinger equation is assumed. The major emphasis of this course is to derive the 'Transition Moment Integral' using semi-classical approach. Further, the relationship between the transition moment integral to experimental observables such as extinction coefficient (from Beer-Lambert law) will be evaluated.

ABOUT INSTRUCTOR :

Prof. G. Naresh Patwari is a professor at the Department of Chemistry, IIT Bombay. After obtaining bachelors from Osmania University in 1992 and master's degrees from University of Hyderabad in 1994, he joined Tata Institute of Fundamental Research for the PhD program and graduated in 2000. A two-year postdoctoral stint at Tohoku University followed by a year at University of Illinois at Urbana Champaign. He joined IIT Bombay in 2003 as assistant professor and became professor in 2012. His research addresses variety of phenomena involving intermolecular interactions using both experimental and theoretical methodologies. Prof. G. Naresh Patwari is the winner of Shanti Swarup Bhatnagar Prize in Chemical Science for the year 2017.

COURSE PLAN :

Week 1: Introduction to Quantum Chemistry; Schrodinger Equation

Week 2: Time Dependent Perturbation Theory

Week 3: Properties of Light

Week 4: Interaction Hamiltonian

Week 5: Transition Probability

Week 6: Einstein A and B Coefficients and Extinction Coefficient

Week 7: Spectral Line-shapes and Lifetime

Week 8: Selection Rules for Rotational, Vibrational and Electronic Transitions