



APPLICATION OF SPECTROSCOPIC METHODS IN MOLECULAR STRUCTURE DETERMINATION

PROF. S. SANKARARAMAN

Department of Chemistry
IIT Madras

PRE-REQUISITES : A good background knowledge in organic chemistry/stereochemistry necessary

INTENDED AUDIENCE : BSc Chemistry final year, MSc Chemistry and PhD Chemistry students.

INDUSTRY SUPPORT : Scientists in Chemical and Pharma industry will be interested. Beneficial to scientists working chemistry in R&D labs, national labs etc

COURSE OUTLINE :

Chemists are molecule makers. Whenever a new molecule is synthesized it is essential to determine its structure using spectroscopic techniques. This course is all about practical applications of spectroscopic methods for the determination of organic molecules.

ABOUT INSTRUCTOR :

Prof. S. Sankararaman has 25 years of teaching and research experience at IIT Madras. He teaches theory courses on organic chemistry, organometallic chemistry, spectroscopy and photochemistry to MSc and PhD students in addition to teaching basic organic and inorganic chemistry courses to B.Tech students. He has written a textbook on Pericyclic Reactions published by Wiley-VCH in 2005. His research interests are in the areas of organic and organometallic chemistry, organic synthesis and catalysis.

COURSE PLAN :

Week 1: Introduction to spectroscopic methods - Nuclear magnetic resonance spectroscopy (NMR), spin $\frac{1}{2}$ nuclei, ^1H and ^{13}C -NMR spectroscopy, FT-NMR method. Chemical shifts, spin spin coupling, spin-spin splitting pattern recognition for structure elucidation, coupling constants.

Week 2: ^1H NMR spectroscopy, Second order effects in NMR spectrum, AB and AA'BB', ABC spin systems. Solving simple structure elucidation problems with ^1H and ^{13}C NMR spectroscopy

Week 3: Stereochemistry determination using NMR techniques. Study of dynamic processes by NMR spectroscopy - examples from organic and organometallic chemistry

Week 4: Mass Spectrometry - various ionization methods - EI, CI, ESI and MALDI methods, fragmentation patterns of simple organic molecules, Use of HRMS.

Week 5: Mass spectrometry - fragmentation patterns of simple organic molecules (continued), solving structure elucidation problems using mass spectrometry.

Week 6: Infra-red spectroscopy - basic concepts, experimental methods, functional group analysis and identification using IR spectroscopy, structural effects on vibrational frequency

Week 7: UV-Vis spectroscopy, electronic transitions in organic molecules, selection rules, application of Beer Lambert law, qualitative and quantitative analysis by UV-Vis spectroscopy.

Week 8: Solving structure elucidation problems using multiple spectroscopic data (NMR, MS, IR and UV-Vis).