APPLICATION OF SPECTROSCOPIC METHODS IN MOLECULAR STRUCTURE DETERMINATION

PROF. S. SANKARARAMAN
Department of Chemistry
IIT Madras

TYPE OF COURSE : Rerun | Elective | UG IPG
COURSE DURATION : 8 weeks (17 Aug' 20 - 9 Oct' 20)
EXAM DATE : 18 Oct 2020

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

INTENDED AUDIENCE : PG and PhD levels

INDUSTRIES APPLICABLE TO : 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 M.Sc. 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 spectroscopy – The electromagnetic spectrum.

Week 1**:** Introduction to magnetic resonance, spin ½ nuclei, 1H and 13C NMR

Week 1**:** Concept of chemical shift, spin-spin coupling

Week 1**:** Structural effects on chemical shifts and coupling constants

Week 1**:** Spectral pattern recognition and structure elucidation of simple molecules

Week 2**:** Second order effects in 1H NMR, simplification methods of second order spectra

Week 3**:** Module 1 and 2: Study of stereochemical aspects by NMR spectroscopy, use of shift reagents, determination of enantiomeric excesses using NMR method

Week 4**:** Structure problem solving using 1H and 13C NMR data

Week 5**:** Module 3, 4 and 5: Fragmentation patterns of simple organic molecules, Retro Diels –Alder fragmentations, type 1 and McLafferty rearrangements, ortho effects.

Week 6**:** Introduction to vibrational (IR) spectroscopy, normal modes of vibrations

Week 7**:** Introduction to UV-Vis spectroscopy, electronic transitions, Frank Condon principle

Week 8**:** All the modules of week 8 will be devoted to problem solving sessions using multiple spectroscopic data involving NMR, MS, IR and UV-Vis