SYMMETRY, STEREOCHEMISTRY AND APPLICATIONS

PROF. ANGSHUMAN ROY CHOUDHURY

Department of Chemical Sciences

IISER Mohali

PRE-REQUISITES : Should have passed 10+2 with science

INTENDED AUDIENCE : 1st and 2nd year B.Sc. students

INDUSTRIES APPLICABLE TO : R&D section of Chemical, Pharmaceutical industry

COURSE OUTLINE :

This course would highlight the concepts and applications of molecular symmetry, isomerism, chirality, applications of stereochemistry in simple organic reactions etc. The students will be introduced to various symmetry elements and symmetry operations observed in various organic molecules, how to identify the symmetry elements and then determine the point groups etc. Then the students would learn the difference between conformation and configuration, various aspects of stereochemistry and will learn to visualize molecules in 3D. Then the course will deal with various organic reactions where stereochemistry plays a major role. This course is suitable for 1st and 2nd year B. Sc students studying Chemistry as one of the subjects in their curriculum.

ABOUT INSTRUCTOR :

Prof. Angshuman Roy Choudhury has obtained his M. Sc degree in Chemistry from Calcutta University in 1999 and Ph. D. from Indian Institute of Science, Bangalore in 2005 working in the area of small molecule X-ray crystallography. Following that he has worked in the University of Liverpool as a post-doctoral fellow from October, 2004 to September, 2007. Then he moved to BITS, Pilani as Assistant Professor in Chemistry. From there, he moved to IISER Mohali in December, 2009 as Assistant Professor in chemistry. He has more than 95 publications in various international journals, guided two Ph. D students and a few masters students at IISER Mohali.

COURSE PLAN :

Week 1: Introduction, IUPAC nomenclature of organic compounds, Conformation and Configuration, Molecular symmetry elements

Week 2: Molecular point groups, Conformational analysis of alkanes and substituted alkanes, Newman and Saw-horse projection

Week 3: Conformation of cyclic molecules: cyclohexane, mono and disubstituted cyclohexane, cyclohexene, cis- and trans- decalene etc

Week 4: Isomerism: Stereoisomerism, topicity of ligands and faces, Enantiomers and Diastereomers, asymmetry and dissymmetry, Fisher Projection

Week 5: Stereoisomerism in chiral molecules- optical isomerism, Circular Dichroism (CD) and Optical Rotatory Dispersion (ORD) and their applications, racemization, D/L and R/S nomenclature, meso-compounds etc.

Week 6: Pseudoasymmetry, Stereochemistry of Allenes, substituted Allenes, Atropeisomerism in Biphenyl and Spiro compounds, Geometrical isomerism (cis-/trans- and E/Z notations)

Week 7: Diastereoisomerism in cyclic system- cyclopropane, cyclobutane, cyclohexane, compounds containing C=O, C=N, fused ring compounds

Week 8: Application of stereochemistry in chemical reactions: Stereoselectivity, Stereospecificity, Regiospecific, Regioselective, Chemoselective reactions Introduction to rate of a reaction, rate determining step etc.

Week 9: Stereochemical aspects of basic organic reactions: SN1, SN2, SNi, NGP, E1 and E2 reaction mechanism, reactions of cyclohexane derivatives

Week 10: Cycloaddition reactions: Diels-Alder reactions, Hydroboration-Oxidation of alkenes,, Baeyer-Villiger Oxidation. Stereochemistry of Aldol condensation, Wittig reaction, Carbonyl addition reaction

Week 11: Stereochemistry of Molecular rearrangements: Pinacol rearrangement, Hoffman, Curtius, Schmidt and Lossen rearrangemnet, Beckmann, Wolff Rearrangement, Cope, Claisen rearrangement

Week 12: Introduction to crystallographic symmetry: 1D symmetry, Concept of 2D symmetry and lattices, notations of symmetry elements, space groups in 2D, 3D lattices, 32 point groups and their notations, crystal systems and Bravais lattices