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## Crystal structure studies of small molecules

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X-ray crystallography is the fastest area of research. Crystal structure analysis has gained its importance during the last few decades due to its intense application in the field of material science and medicine particularly in the drug industry. The characterization of materials which are biologically interesting is important and hence the technique of single crystal X-ray diffractometry has gained prominence. The X-ray studies thus play an important role in the design of appropriate drugs. More interest would be focused on co-crystals, hydrogen bonding, polymorphism, pseudopolymorhism, and disorder studies. Crystallographic studies on the structure, symmetry, and confirmation of some organic molecules of wide interest and fundamentals of crystallography form the basis of the present lecture. Single crystal x-ray diffraction is the most common experimental method of obtaining a detailed picture of a large molecule that allows resolution of individual atoms. It is performed by analyzing the diffraction of x-rays from an ordered array of many identical molecules. Many molecular substances, including proteins, polymers, and others solidify into crystals under the proper conditions. When solidifying into the crystalline state, these individual molecules typically adopt one of only a few possible orientations. A crystal is a three-dimensional array of that are held together by Vander Waals, non-covalent bonding. The smallest representative unit of crystals is referred to as the unit cell. Understanding the unit cell of these arrays simplifies the understanding of a crystal as a whole. This is the basis of crystallography. Many organic compounds with pharmaceutical importance exhibits polymorphism. Polymorphism, the ability of a substance to exist in several different crystal forms or modifications, is a frequently observed phenomenon in molecular compounds. If a solid substance includes a solvent during crystallization, this structure is known as a pseudopolymorph, and in case of, e.g., water such crystal forms are generally called hydrates. The polymorphic modifications of a compound are chemically identical but usually differ in their physical and chemical properties, such as density, vibrational spectra, and diffraction patterns. Co-crystals are a crystalline material composed of different species held together by non-covalent forces and are typically differentiated from a salt by the lack of proton transfer. Co-crystals offer the framework to modify the physical properties of the compounds involved without changing the molecular structure. Pharmaceutical co-crystals have become increasingly important materials because of their potential to improve the physical and chemical stability of the compounds involved, decrease hygroscopicity of the crystalline material, increase the kinetic or thermodynamic solubility of the compounds or modify dissolution rates for a compound. Therefore, it is really worthwhile to study the crystal and molecular structure studies of various organic compounds and find exactly what type of interactions are present in these molecules. These interactions would be helpful to understand the biological studies or activity of these molecules.

### Biography

Hemmige Yathirajan has worked for nearly 42 years in the DOS in Chemistry, University of Mysore, Mysore, India as a teacher and researcher. His main area of research is x-ray crystallography and deals with small molecules. He has worldwide collaboration in this area of research and has about 750 research publications.

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