X-Ray Crystallography Encyclopedia Article

X-Ray Crystallography

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X-Ray Crystallography

X-ray **Crystallography** is the study and determination of crystalline structures through x-ray diffraction techniques. In 1953, Watson and Crick used x-ray crystallography to discover the double-helix structure of **DNA**. X-ray crystallography is most commonly used in biological and medicinal fields to determine the structures of complex proteins. The protein structures are invaluable in drug and medicine research, resulting in advances in treatment and more efficient production of pharmaceuticals.

The first step in an x-ray diffraction experiment is to grow crystals of the molecule being studied. Several methods are available for growing crystals, the most common being vapor diffusion. Other approaches currently in use are macroseeding, microseeding, batch crystallization, microbatch crystallization, free interface diffusion, and dialysis. To yield crystals of the desired size, several techniques are used in any one diffraction experiment because of the extreme difficulty in controlling the crystal formation.

When electromagnetic waves of an exceedingly small wavelength (comparable to the size of the molecule's bonds) are passed through a molecule, the waves are diffracted by the electron clouds of the constituent atoms. The diffraction is amplified greatly because of the crystal's characteristic repetition of structure. If there were a way to focus x rays, an x-ray "picture" could be produced from these diffraction patterns. However, because x rays are so penetrative, focusing them is impossible. To provide a picture of the individual atoms on such a small scale, the patterns of interference must be recorded and thoroughly analyzed. The diffraction patterns produced can be used by computers to create electron density maps that show the electron probability distribution of the molecule in a topological style. The relative positions of atoms in a molecule can be determined because electrons are most densely packed around the atom's **nucleus**. One problem of this approach is that atoms of hydrogen, with only one electron, are very hard to pinpoint. Using electron density maps, a 2-D picture of the molecule is generated. To extrapolate a 3-D structure from the diffraction patterns, the experiment is repeated through small increments in the angle of the crystal's rotation with respect to the x-rays. Using many electron density maps, and watching how they change, scientists can find a relative 3-D orientation for each atom within the crystal.