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Molecules and Crystals, 1926—1970

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(The full text of the lecture is published in Helvetica Chimica Acta)

Summary

The history and development of X-ray crystallography is described, with special reference to the structure of organic molecules. During the 1920's and early 1930's a small number of fundamental structures was elucidated, but the work was slow and laborious. Phase determining methods based on the use of heavy atoms and isomorphous replacement were then developed in the course of the phthalocyanine work (1935–1940) and this provided the key for solving structures of unknown chemical constitution, no matter how complex. But the work was still slow and difficult owing to the magnitude of the computations involved. However, a number of important and heroic determinations of complex organic structures was soon accomplished, including cholesterol and calciferol derivatives, strychnine and other alkaloids, limonin, penicillin and vitamin B_{12}.

The next great advance in crystallography began with the invention of the electronic digital computer, which became available in the later 1950's and 1960's. This has removed the computational burden, and complex structure determinations can now be completed in weeks instead of in years. The output of new structures is now so enormous that no summary is possible, and the results are transforming the science of chemistry.

Within the last 10 years the methods of crystallography have been successfully applied to a large number of important biological molecules, the proteins and enzymes. About 30 of these giant molecules, containing thousands of atoms, have now been solved in detail and the positions of most of the atoms determined. In every case the methods employed to solve the phase problem were those involving the use of heavy atoms and isomorphous replacement. These results have now enabled the mechanism of enzyme action to be studied in detail for the first time, and they are rapidly increasing our knowledge of biological processes at the atomic and molecular level.