P-1 10:00 ~ 10:40 Plenary Talk I

Phase Problems in Crystallography

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The object of a crystal-structure determination is to locate the atomic positions within the unit cell by tackling the phase problems and thus completely to define the whole structure.

The earliest method for solving crystal structures was by a process of trial and error. Possible structures were postulated and the calculated and observed intensities compared in order to test the plausibility of the postulates. There could be no quarrel with calling such a method indirect.

The advent of the Patterson function marked an important advance. An examination of the vector map, coupled perhaps with chemical knowledge, may yield important information concerning the orientation or relative position of groups of atoms or even enable a complete structure determination to be made. A Fourier synthesis, calculated with the observed structure amplitudes with phases given by the contributions of the heavy atoms, will then often show the electron density associated with the remaining atoms of the structure. In such a case the structure may be considered to have been determined directly, in the sense that a routine series of operations has led from the diffraction data to the structure.

The adjective "direct", however, is usually reserved for those methods which attempt to derive the phases of the structure factors directly by mathematical means from the X-ray diffraction data. Direct methods are usually cast in the form of a mathematical problem which, once formulated, may be solved by a routine sequence of steps in which any decisions are of a purely mathematical nature.

Currently the direct methods are effective enough in their way, but, from the educational point of view, they are poor fodder for the trainee crystallographer because ever faster computers undertake to execute all the processes from obtaining the X-ray data to arriving at the final solution numerically.