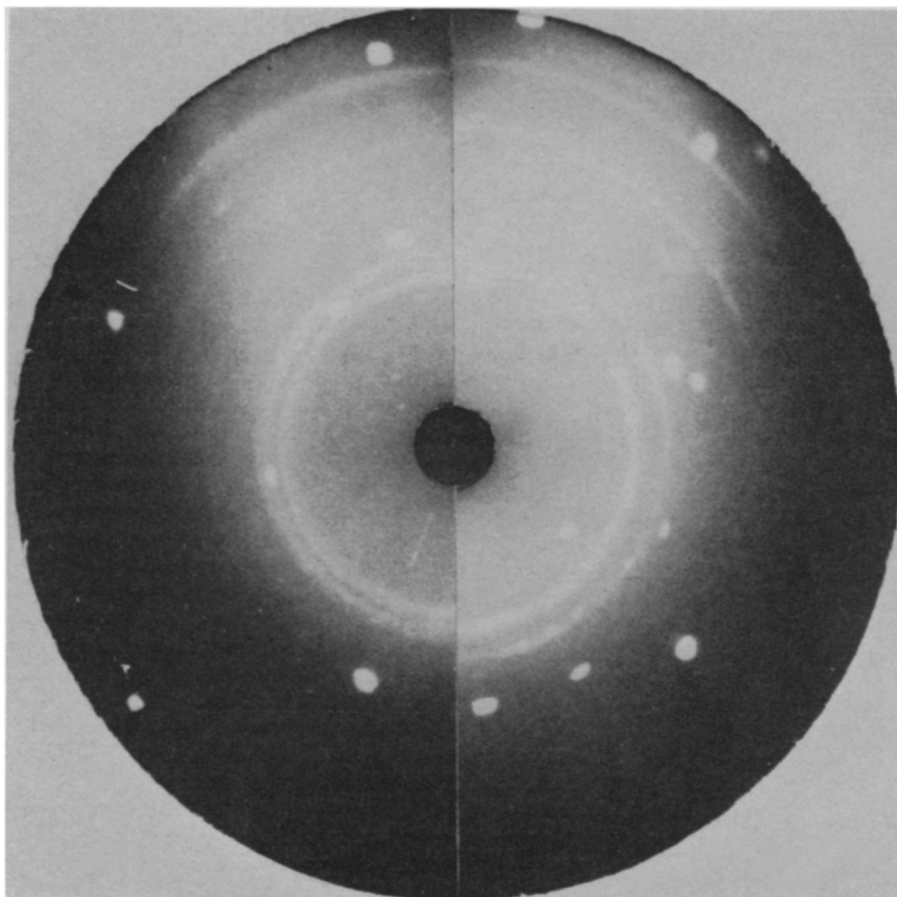


*Diffraction patterns of hexagonal thallium (right) under different pressures. Left half shows pattern at one bar; right at 60 kilobars.*



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#### CRYSTALLOGRAPHY

## An old science retains a spark

**Techniques fully developed;  
It now remains only to put them to full use**

by Barbara J. Culliton

To explain and perhaps alter the physical and chemical properties of solid matter, from metals and alloys to hormones, proteins and nucleic acid, scientists must know exactly how atoms are positioned within crystals. Elucidating this structure is the province of crystallographers whose primary tools are crystal-penetrating X-rays.

**X-ray crystallography**, which has been around since early in the century, spent much of its infancy in Europe, particularly in Germany and in France. There, for 30 years, Dr. Andre Guinier, known particularly for his contributions to the development of small-angle scattering, worked to perfect various techniques of bombarding crystals and measuring the intensity and direction of scattered X-ray. Since the amount the X-rays are bent depends on how far apart layers of atoms in the crystal are, the scatter pattern shows the structure of the crystal.

Despite the age of the discipline, the August meeting of the American Crystallographic Association in Buffalo was charged with an air of exuberance usually reserved for a new science. The atmosphere was not the least subdued when Dr. Guinier proclaimed, for example, that "the theory of small-angle scattering seems to have reached its limits. There is no hope to go further."

His statement reflects the fact that crystallography, which for years con-

cerned itself with methodology, has come of age. As Dr. Guinier put it, "now interest is in application, not in the progress of technique."

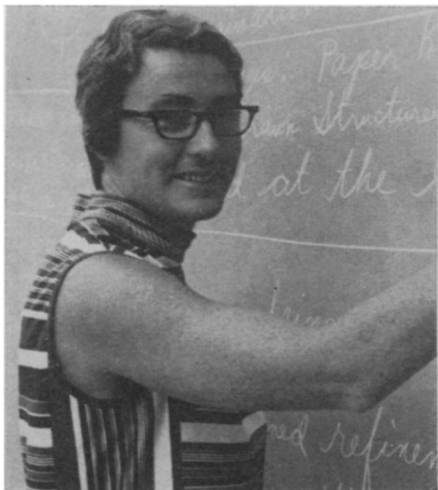
The way is now open to scientists who envision new uses of metals and, particularly, to biologists who see in crystallography a route to the solution of problems difficult for even the most sophisticated chemistry.

Three years ago Buffalo's Roswell Park Memorial Institute opened its Center for Crystallographic Research. Its director, Dr. David Harker, announced last year the complete three-dimensional structure of ribonuclease, the third protein to be analyzed completely (SN: 2/4/67, p. 119). He had begun analysis of this protein, essential to all protein synthesis, in 1950, making some 60,000 measurements of ribonuclease crystals before deciphering the structure. "To understand behavioral properties," he says, "we want to learn the detailed geometrical biochemistry of cells."

**Now, according to** Dr. Dorita Norton of the Medical Foundation of Buffalo and chairman of the meeting, the day of such time-consuming work is past. Computers, hooked into sophisticated X-ray cameras (one was developed by Dr. Harker), make it possible to get the structure of a small molecule in about four weeks, she estimates. In her own work on hormones, aimed at



Pioneers: Drs. Harker (right) and Guinier, between sessions at Buffalo.



Dr. Norton makes a point.



Photos: Don Glenna

Watching a science shift gears.

finding out how they work, it takes about three months to determine the configuration of a 60-atom molecule. A larger molecule, such as a protein containing 2,000 to 3,000 atoms, can be analyzed in one or two years, compared to Dr. Harker's 17.

"X-ray crystallography is doing what a lot of people hoped the electron microscope would do when it came along in the 1950's," says Dr. Donald F. Parsons of Roswell Park.

Dr. Parsons is using crystallographic techniques on proteins, hoping that known atomic structure will explain how a protein fits into a cell membrane. Membranes have a gate function, regulating what goes in and what goes out of a cell, and therefore how it behaves. Although specific points of variation remain unknown, researchers do know that cancer cell membranes differ from normal membranes in a tool for exploring this phenomenon," he says.

Crystallography's role in the potential expansion of knowledge about proteins

is matched by its place in the study of nucleic acids. James D. Watson and Francis H. C. Crick won the Nobel Prize with their construction of the double stranded helical configuration of DNA (deoxyribonucleic acid). Their work, crystallographers are quick to point out with pride, would not have been possible without the crystallography, for which Maurice H. F. Wilkins shared the prize.

Yet for all that is known about DNA and RNA (ribonucleic acid), "nucleic acid research is not over; it's really just beginning," says Dr. Muttaiya Sundaralingam of Case Western Reserve University in Cleveland. "Much of the work proving the structure of nucleic acids so far is based on fitting a few observations to theory derived from chemical evidence. Though the evidence is convincing, we're trying to prove what a chemist can only postulate by identifying the crystalline structure, not of the whole DNA or RNA macromolecule, but of its components, the smaller nucleotides and nucleosides." ◇

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