

Herbert Aaron Hauptman

Mathematician and crystallographer Herbert Aaron Hauptman died on 23 October 2011 in Buffalo, New York, at the age of 94. Herb, as he was known by his friends and colleagues, was a co-recipient, with Jerome Karle, of the 1985 Nobel Prize in Chemistry for developing mathematical methods to determine crystal structures.

Herb was born in New York City on 14 February 1917. He later credited his parents for aiding his development as a scientist by allowing him to pursue subjects of his own choosing. In his Nobel autobiography he wrote, "My interest in most areas of science and mathematics began at an early age, as soon as I had learned to read, and continues to this day."

Herb grew up in the Bronx and attended Townsend Harris High School, where his interest in science and mathematics was nurtured. He continued his studies at the City College of New York and graduated in 1937; he received the Belden Medal as the top student in mathematics. He also earned a master's degree in mathematics at Columbia University in 1939.

Soon after he and Edith Citrynell married in 1940, they moved to Washington, DC, where Herb worked for two years as a statistician at the US Census Bureau.

In 1942 Herb joined the legions of young Americans who served in World War II. A Navy ensign, he was stationed in the Southwest Pacific. Although he only had one day of firefighter training, he was a fire marshal in the Philippines—an assignment that twice nearly cost him his life. To help keep his mind sharp during the war years, he spent his rare moments of spare time studying calculus and solving mathematical problems. His wartime experience led him in future years to protest actively against US involvement in other military actions, including the Vietnam War.

After World War II, Herb began collaborating with Karle at the US Naval Research Laboratory (NRL). Coincidentally, Karle was also a 1937 graduate of the City College of New York. Herb's background in mathematics and Karle's in physical chemistry complemented each other nicely, and together they started research on the phase problem of x-ray crystallography, which had daunted other scientists for decades. At the same time, Herb enrolled in the doctoral program in mathematics at the University of Maryland, where he completed his dissertation, "An n -dimensional Euclidean algorithm," in 1955 under the direction of Richard Good.

The diffraction pattern that is formed when x rays pass through a crystal depends on the positions of the atoms in the crystal. However, in the early 1950s it was difficult or impossible to work backwards from the diffraction data to the atomic arrangement because only the intensities, and not the phases, of the diffracted x rays could be measured experimentally. Herb and Karle used probability theory—in particular the joint probability distribution of several structure factors—to

develop mathematical techniques, called direct methods, to find the phases of some of the x-ray reflections leading ultimately to an entire three-dimensional molecular structure. During the past half century, direct methods have facilitated the determination of many thousands of crystal structures important to medicine and numerous other disciplines.

The main ideas of Herb and Karle's direct methods were published in 1953 in their American Crystallographic Association (ACA) monograph entitled *Solution of the Phase Problem I: The Centrosymmetric Crystal*. However, direct methods were largely ignored for at least a decade, not only because they were poorly understood but also because the necessary computations were laborious. The development of better computers and more sophisticated programs eventually led to acceptance and widespread use of the methods and culminated in Herb and Karle receiving the ACA Patterson Award in 1984 and, finally, the Nobel Prize in 1985.

By the late 1960s, Herb was head of the NRL's mathematical physics department. But in 1970, unwilling to shift the focus of his naval research to laser-guided missiles, he seized the opportunity to join the crystallographic group of a small, nonprofit biomedical research institute, the Medical Foundation of Buffalo. In 1972 he became the MFB's research director; he later became its president. In 1994 the MFB was renamed the Hauptman-Woodward Medical Research Institute (HWI) to honor him and Helen Woodward Rivas, the philanthropist who provided the seed funds for it.

During his years in Buffalo, Herb also was a professor in the departments of structural biology, biophysical sciences, and computer science at the University at Buffalo. Throughout his career he was a mentor to aspiring crystallographers around the world and taught at



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many International Union of Crystallography computing schools, at Erice conferences in Italy, and at specialized meetings dedicated to direct methods.

The direct methods for which Herb shared the Nobel Prize began to break down for structures with more than 100 nonhydrogen atoms. Therefore, during the 1990s he led his Buffalo colleagues in extending the range of those methods. The result was a new, more powerful version of direct methods, known as shake-and-bake, that repeatedly alternates phase refinement with the imposition of physical constraints. Shake-and-bake can be applied successfully to structures 10 times as large. In addition, direct methods can now be used routinely to determine large heavy-atom substructures of proteins.

Herb continued to work daily at the HWI into his nineties. He received his last research grant at age 89 from the Human Frontier Science Program for a study of structure determination using neutron diffraction data.

Herb loved to hike in the Blue Ridge Mountains of Virginia, listen to classical music, and design and make beautiful stained glass stellations of the Platonic solids, such as the ones seen in the photo. All of us at the HWI will miss his guiding spirit. He was not only a superb scientist, mentor, and colleague but also a wonderful friend.

Charles M. Weeks

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